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AIR MONITOR SITING BY OBJECTIVE

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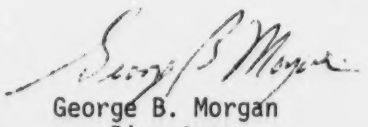
FOREWORD

Protection of the environment requires effective regulatory actions which are based on sound technical and scientific information. This information must include the quantitative description and linking of pollutant sources, transport mechanisms, interactions, and resulting effects on man and his environment. Because of the complexities involved, assessment of specific pollutants in the environment requires a total systems approach which transcends the media of air, water, and land. The Environmental Monitoring and Support Laboratory-Las Vegas contributes to the formation and enhancement of a sound monitoring data base for exposure assessment through programs designed to:

- develop and optimize systems and strategies for monitoring pollutants and their impact on the environment.
- demonstrate new monitoring systems and technologies by applying them to fulfill special monitoring needs of the Agency's operating programs.

This report discusses the theoretical basis for a method of designing air quality monitoring networks with regard to the specific objective(s) of the network. The method is presently only applicable to nonreactive pollutants and requires the existence of limited air quality monitoring data. Regional and local agencies may find this method useful in planning or adjusting their air quality monitoring networks. The Monitoring Systems Design and Analysis Staff may be contacted for further information on the subject.



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A method is developed whereby measured pollutant concentrations can be used in conjunction with a mathematical air quality model to estimate the full spatial and temporal concentration distributions of the pollutants over a given region. The method is based on the application of estimation theory to systems described by partial differential equations, such as the atmospheric diffusion equation. A computer code has been developed that can process monitoring data to produce concentration distribution estimates. The code has been tested extensively on a hypothetical airshed, designed to illustrate the key features of the method. Once concentration distributions have been estimated, new monitoring stations can be located based on several siting criteria.

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SECTION 1

INTRODUCTION

Urban air pollutant monitoring systems consist of an array of stations located throughout the region at which pollutant concentrations are measured continuously or intermittently. At present in most systems the data are transmitted to a central facility and stored for possible future use. The object of this study is to develop a methodology by which air monitoring data from an urban monitoring system may be processed in real time to produce continuous estimates of the spatial and temporal concentration distributions of pollutants over a region, and thereby to locate pollutant maxima under various meteorological conditions.

Mathematical urban air pollution models enable the prediction of the spatial and temporal concentration distributions of pollutants under varying meteorological and source emission conditions. Given a region with no monitoring stations it is possible to estimate pollutant concentration distributions in the airshed as long as pollutant source emissions and meteorological data are available. In such a case it is possible to perform numerical experiments with a mathematical model under various source and meteorological conditions to find the locations of the highest concentrations of particular pollutants and then to design a network initially for the region based on these predicted pollutant concentrations.

The more common situation is that in which several monitoring stations are already in existence in a region. In addition to routine surveillance it may be desired either to move those stations or to place new stations within the region. In such a case, it is desirable to use the information available from the existing stations as well as the information that can be obtained by exercising a mathematical model. The basic problem involved is that of coordinating in a consistent manner the measurements available from the stations and the predictions of the mathematical model. The development of a framework for this integration is the object of this work. Thus, our objective is to develop means by which urban air pollution models can be used together with air monitoring data to estimate the complete spatial and temporal concentration distributions over a region. As noted above, if this can be done, then additional stations can be located or existing stations can be moved for better or more effective surveillance of pollutant concentrations. In Section II we cite several objectives by which one would locate stations. Each of these objectives can be met if one has the knowledge of concentration distributions over the whole region and how the concentration distributions vary with changes in meteorology and sources.

The basic problem we consider, therefore, is the use of data from an existing monitoring network in conjunction with an air quality simulation model to produce estimates of pollutant concentrations over the entire region. Thus, we are developing a means by which point data can be used in conjunction with a mathematical model to produce area-wide concentration distributions as a function of time. This is essentially an optimization problem in that we want to estimate that concentration distribution that is as close as possible to both the monitoring data and the mathematical model. Because of inherent fluctuations in atmospheric measurements and because mathematical models are inexact, there will never be complete agreement between model predictions and measured data.

The optimization problem associated with estimating concentration distributions is formulated and solved. The main consideration in implementing the theory is the computational requirements. In short, the solution requires the solution of an equation similar to the mathematical model for the estimated concentrations and of an additional set of equations for the statistics (variances) of the concentration estimates. The equations for the variances are cumbersome. A significant portion of the present study has been devoted to determining the most efficient numerical way to implement the model and variance equations so that ultimately the algorithm can be exercised by the U.S. Environmental Protection Agency (EPA) with reasonable amounts of computing time for an urban region. In this report we describe a systematic investigation of each of the available numerical approximate methods for solution of the model and variance equations. We present a computer program capable of producing concentration estimates from an arbitrary number of monitoring points in a given region with a 3-dimensional model. The program is structured in a general way for a 2-dimensional wind field, vertical diffusivity, and source emissions, and an arbitrary number of monitoring locations. The program will, given measurements of pollutant concentrations, produce estimates of the full concentration distribution over the region. In its present version the program relates only to inert pollutants and does not include a vertical component in the wind field. Such conditions could be added if a comprehensive air quality simulation model were to be integrated into this routine.

SECTION II

DESIGN OF A MONITORING SYSTEM

Monitoring ambient air quality is an indispensable, and perhaps the single most important, activity in the evaluation and control of air pollution. Without reliable measured data, one cannot establish a quantitative relationship between atmospheric pollutant levels and source emissions, nor can one assess the effects of polluted air on man and his environment.

With the passage of the Clean Air Act, including the 1977 amendments, ambient air monitoring programs have become an essential part of state implementation plans. In its 1975 document on design of air monitoring networks, EPA states that "much more consideration, in both manpower and monetary resources, should be applied to the issue of siting monitoring facilities than is currently the common practice... It is considered inconsistent to undertake a monitoring effort involving resources in the tens of thousands of dollars without investigating the far smaller effort involved in... proper siting of the monitoring instruments." (Environmental Protection Agency, 1975.)

The design of an ambient air quality monitoring network will depend on the purpose of the network. The following general monitoring objectives have been delineated by the EPA:

(1) To establish a basis for comparison of air quality standards with actual air quality levels, to measure progress toward compliance, and to establish the degree to which compliance is achieved.

(2) To provide a basis for ascertaining long term trends. (The implementation of most air pollution control strategies takes time. The effectiveness of these strategies, as reflected by the gradual changes in air quality, can be evaluated only through careful comparisons of historical records of air quality data.)

(3) To provide air quality data during episodes

(4) To monitor source compliance with regulations

(5) To provide data to support enforcement actions

(6) To provide data for research.

The development of a permanent air quality monitoring network involves the determination of the number and location of sampling sites, selection of appropriate instrumentation, determination of the frequency and schedule of

sampling, and establishment of instrument and probe siting criteria (Environmental Protection Agency, 1975). In this work we confine our attention to the first aspect, namely the determination of the number and location of sampling sites. As noted above, the configuration of an air quality monitoring network involves two elements--the number of sensors and their geographical location. Decisions on the two elements can be made in either order, that is, the number of stations can be prescribed based on a criterion of cost and then distributed geographically in some optimal fashion, or the number of stations and their locations may be chosen on the basis of the monitoring criteria. The minimally required number of monitoring stations can be judged, in general, from factors such as the absolute levels of pollutant concentrations, the variability of the spatial concentration distribution, and the physical size and population distribution of the region.

Air pollutants are emitted from a variety of sources and are transported and dispersed by an atmosphere, the turbulent processes in which can only be described statistically. As a result, pollutant concentrations not only fluctuate in time; they generally differ from place to place as well. The most difficult question confronting a designer of monitoring systems can be therefore expressed as: "Where in this highly variable field should the stations be placed so that representative samples can be collected?" Clearly, an answer lies in the thorough understanding of parameters that can affect the spatial distribution of air pollutants. A variety of non-technical considerations will influence the choice of where to locate monitoring stations, including the security of the site, its accessibility, the availability of utilities, the ability to accommodate future modifications or expansions, and the availability of the site. Harrison (1972) has noted that the prime consideration in selecting sites for the Chicago air monitoring network is security.

A. MONITORING REQUIREMENTS OF DIFFERENT POLLUTANTS

The pollutants commonly monitored in an urban area are carbon monoxide (CO), sulfur dioxide (SO_2), total hydrocarbons, oxides of nitrogen ($NO + NO_2$), oxidant, and total suspended particulate matter. Each has certain atmospheric characteristics that suggest different monitoring requirements.

Carbon monoxide is essentially a non-reactive pollutant generated by motor vehicles. The highest concentrations of CO are observed in urban areas near roadways carrying high volumes of traffic (Chang and Weinstock, 1973). In order to ascertain whether air quality standards for CO are being met, it is therefore most important to monitor in the regions of highest traffic densities. In assessing long term trends it may also be desirable to measure CO at points removed from roadways as well as near roadways. According to recent EPA guidance on siting of CO monitors, six types of sites are discussed and assigned the priorities shown below (Environmental Protection Agency, 1975):

Type of site	Priority
Peak street canyon	1
Peak neighborhood	1
Average street canyon	2

Type of site	Priority
Corridor	3
Background	4
Average Neighborhood	5

Ott and Eliassen (1973) have suggested that present patterns in the siting of stations for CO measurement may not permit adequate assessment of compliance with air quality standards. Ott (1971) conducted a comprehensive survey of air quality (for CO) in the vicinity of a single monitoring station in San Jose, California. Samples were collected along the sidewalk at "breathing level" while walking at random spatially over a specified grid, and in specially prescribed patterns near the station. Ott found that concentrations significantly higher than those recorded at the monitoring station prevailed along the sidewalks of downtown San Jose streets and that these concentrations showed little correlation with values recorded at the station. Near-street measured values (long-term averages) were on the order of a factor of two greater than values recorded at the station.

Ott (1975) has attempted to formulate a set of uniform criteria for CO monitoring. He suggests a dual monitoring approach, in which two monitoring stations are used continuously in each area of the region, one to monitor the lower urban neighborhood concentration and one to monitor the higher concentrations to which pedestrians are exposed near traffic. Ludwig and Keoloha (1975) have suggested procedures for selecting CO monitoring sites representative of downtown street canyon areas, along major traffic corridors, and urban neighborhoods. They make specific recommendations for the heights of monitoring ports, distances from major and minor roadways, and placement relative to urban areas.

Sulfur dioxide is emitted from fossil fuel combustion in power plants and space heating units and from certain industrial operations. Once emitted, SO_2 is oxidized to sulfates on a time scale the order of hours, with substantial amounts of the original gaseous sulfur ending up in airborne particles. Because of the nature of its sources, SO_2 is usually emitted above ground level from stacks or from the tops of buildings. Highest concentrations might be expected to occur therefore at rooftop levels directly downwind of major sources. There is mounting evidence that the most serious SO_2-related health effects are those resulting from exposure to sulfate-bearing particulate matter. These effects would be manifest most strongly well downwind of the SO_2 sources themselves, since time is required to convert gaseous SO_2 to particulate sulfate. With the exception of monitoring downwind of certain strong sources of SO_2, such as a power plant, monitoring requirements for SO_2 suggest area-wide measurements.

Hydrocarbons are emitted from motor vehicles and a large number of industrial sources. There are currently no air quality standards for hydrocarbons based on health effects, although there does exist a standard of 0.24 ppmC (parts-per-million of carbon) for a 3-hour average based on subsequent oxidant formation. There is no need therefore to measure hydrocarbons for possible health effects. The primary reason for monitoring hydrocarbon concentrations is based on the relationship of hydrocarbon levels to oxidant formation.

The oxides of nitrogen, NO and NO_2, have rather different spatial distributions in the atmosphere when there are appreciable emissions of NO. Nitric oxide (NO) is emitted from motor vehicles and stationary combustion operations and can be classed as a primary pollutant. Its highest concentrations can be expected to occur in the vicinity of sources, particularly near heavily travelled roadways. As in the case of hydrocarbons, there is currently no health standard for NO. Nitrogen dioxide (NO_2) is almost totally an oxidation product of NO. A health standard does exist for NO_2 (0.05 ppm annual average) so that measurement to assess compliance with the standard is necessary. Since NO_2 is formed in the atmosphere from NO only after the NO has been mixed with emitted hydrocarbons and allowed to react for a period of an hour or so, local hot spots of NO_2 are not to be expected. Area-wide monitoring at locations downwind of main NO sources is the basic strategy called for.

Photochemical oxidant, primarily ozone, is the major product in photochemical smog. Oxidant forms during prolonged irradiation of hydrocarbon/NO_x mixtures, usually well downwind of where the hydrocarbons and NO were emitted. Clearly, area-wide monitoring is suggested for oxidant, with one proviso. Ozone reacts very quickly with NO. Thus, in the vicinity of local sources of NO, such as roadways, ozone levels are generally significantly depressed relative to ambient levels due to rapid scavenging by NO. Thus, it is necessary to locate monitors for oxidant beyond the immediate vicinity of NO sources.

The final category of pollutant routinely measured in urban areas is total suspended particulate matter (TSP). Particulate matter is emitted from a wide variety of sources, and the monitoring needs of a region will be dictated somewhat by the major sources of particulate matter in that region. Primary particulate matter is emitted from motor vehicles, aircraft, power plants, and industrial operations. The largest particles generally settle out rapidly near the sources, whereas those in the micrometer range and smaller become airborne for relatively long periods of time.

The brief discussion above leads one to the conclusion that it is possible to identify two basic types of monitoring sites, *proximate* and *urban* level. Proximate sites refer to those situated in the immediate vicinity of a source, and are of primary interest in the measurement of CO. In those instances in which significant SO_2 emissions occur from a single source, proximate monitoring may also be called for. The selection of proximate sites will depend on the particular source, its configuration and the local topography. Sources for which proximate monitoring may be necessary are elevated and depressed roadways, street canyons, airports, and perimeters of power plants. The site is to be chosen at the point when the highest concentration levels are expected to occur. A detailed consideration of the selection of proximate sites for CO monitoring has been carried out by Ludwig and Kealoha (1975).

Urban level sites are used to enable the estimation of concentrations of pollutants over broad areas of the entire region or certain subareas of the region. Thus, these sites should be reasonably removed from strong local sources so that each station provides data representative of the "region" of

the airshed in the vicinity of the station. In most cases, "airsheds" have been designated by legislation. As a practical matter, an airshed can be considered as that region in which pollutant concentrations are largely the result of emissions in the airshed. The airshed is usually defined as a region large enough so that a different "airshed" need not be defined for each pollutant. Urban level sites are the type called for, in general, in measurement of SO_2, hydrocarbons, NO_x, oxidant, and particulate matter.

B. SITING CRITERION

Certain objectives of monitoring have been delineated above. Table 1 indicates the various criteria one would consider in attempting to meet the six objectives. Based on Table 1 we can summarize the following criteria for siting of monitoring stations:

(1) Locate stations so that the pollutant concentration distribution over the region can be estimated most accurately.

(2) Locate stations where the expected frequencies of violation of the air quality standards are highest.

(3) Locate stations at points of maximum sensitivity of the pollutant concentrations to source parameters.

The problem of siting on the basis of maximum sensitivity of concentrations to source emission level changes has been considered previously (Seinfeld, 1972). We do not consider this approach in the present work. We choose to focus on the objective of ascertaining compliance with regulations, the most important objective of air quality monitoring. Thus, the criterion with which we will be concerned is to locate stations to enable the best estimation of pollutant concentration distributions over the region, a criterion that includes detection of the places of greatest expected violation of standards.

The criterion of locating stations so that optimal estimates of the full concentration distribution over the region can be obtained is compatible with other criteria being considered by the EPA's Environmental Monitoring and Support Laboratory-Las Vegas (EMSL-LV). For example, in Liu et al. (1977) a Figure of Merit, F, was defined as the product of an air quality index (either observed or predicted) at a particular location and the associated frequency or probability of occurrence,

$$F = \sum (\text{Air Quality Index}) \cdot (\text{Frequency of Occurrence})$$

The summation is to be performed over all meteorological scenarios that lead to air pollution episodes. The Figure of Merit is weighted by the frequencies of occurrence of the scenarios because the pollutant concentration at any location varies significantly over a year, e.g.,McElroy et al. (1978).

$$F(i,j) = \sum_{\ell=1} \left(\begin{array}{l}\text{Frequency of Occurrence} \\ \text{of Meteorological} \\ \text{Pattern } \ell\end{array} \right) \cdot \left(\begin{array}{l}\text{Max. 1-hr. or 8-hr. surface} \\ \text{CO Concentration at} \\ \text{Grid Point i,j under} \\ \text{Pattern } \ell\end{array} \right)$$

TABLE 1. SITING CRITERIA FOR DIFFERENT OBJECTIVES FOR MONITORING

Monitoring Objective	Siting Criterion
1. Assess compliance with air quality standards	Locate stations where concentrations are expected to be largest or locate stations where the spatial concentration distributions can be estimated most accurately.
2. Assess long-term trends	Locate stations where concentrations are expected to be largest or locate stations where the spatial concentration distributions can be estimated most accurately.
3. Provide data during episodes	Locate stations where concentrations are expected to be largest under conditions of stagnation or locate stations where the spatial concentration distributions can be estimated most accurately.
4. Monitor source compliance with regulations	Locate stations at points where the sensitivity of concentration levels to source emission level changes is greatest.
5. Provide data to support enforcement actions	Locate stations at points where the sensitivity of concentration levels to source emission level changes is greatest.
6. Provide data for research	For the evaluation of diffusion models, locate stations where the spatial concentration distributions can be estimated most accurately.

In this approach, McElroy et al. (1977), the CO concentration is predicted by an urban air pollution model for each situation corresponding to the various meteorological patterns. Air quality data are not necessary to implement that approach (only, of course, for the validation of the air quality model); with source emission and meteorological inputs the concentrations can be predicted in the absence of air monitoring data. When there are no air monitoring stations in a region then the technique of Liu et al. (1977) must be used. The approach that we have chosen to follow is based on the availability of air monitoring data. In short, we seek to utilize past air monitoring data to estimate the full pollutant concentration distribution over the region. Once this distribution has been estimated, then the Figure of Merit can be computed. Our approach recognizes, therefore, the fact that air quality model predictions will not perfectly match ambient data and attempts to reconcile the model predictions and the data to produce an "optimum" estimated concentration distribution.

SECTION III

OPTIMAL ESTIMATION OF AIR POLLUTANT CONCENTRATIONS

In Section II we discussed several objectives of monitoring and the resultant siting criteria. We arrived at the criterion of locating stations to enable the optimal estimation of pollutant concentration distributions over the region as one that satisfies many of the principal objectives of monitoring. In this section we outline the theory underlying the implementation of this criterion.

A. MATHEMATICAL MODELS OF URBAN AIR POLLUTION

In attempting to quantify the siting criterion and determine an optimum design it will be necessary to employ a model that relates emissions to air quality. Models of this type can be classified as *dynamic* or *long-term*. Dynamic models describe the evolution of pollutant concentrations in the region during a day, given source emission and meteorological information. Long-term models predict the yearly average pollutant concentrations as a function of location in the airshed and incorporate information on the frequencies of occurrence of various meteorological conditions in the region over a typical year (Kumar et al., 1976). The monitoring location problem can be formulated on the basis of the dynamic behavior of pollutants on typical days (requiring the use of a dynamic model) or on the basis of the long-term, average concentration distributions over the region (necessitating the use of long-term models). Since dynamic models, if accurate, incorporate much more detail than long-term models, particularly when episode conditions are of interest, siting on the basis of the dynamic behavior of pollutants is preferable to that based on long-term averages. Consequently, we confine our attention here to siting on the basis of dynamic behavior. For an example of an approach to monitor siting based on long-term averages we refer the reader to Darby et al. (1974).

All conventional atmospheric diffusion models are based on the equation of conservation of mass

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} + v\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = \mathcal{D}_i\left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2}\right) + R_i(c_1,\ldots,c_N,T) + S_i(x,y,z,t) \qquad (1)$$

where c_i is the concentration of species i; u, v, and w are the fluid velocities in the three coordinate directions; $\mathcal{D}_i$ is the molecular diffusivity of species i in air; R_i is the rate of generation (or the negative of the rate

of disappearance) of species i by chemical reactions at temperature T; and S_i is the rate of injection of species i into the fluid from sources.

Because the atmosphere is a turbulent flow, the velocities u, v, and w are random functions of space and time. Consequently, the concentration c_i is also a random function of space and time. Solutions of (1) with realistic atmospheric velocities are very difficult to obtain, even in the case in which $R_i = 0$ (inert species). In order to render (1) solvable, the fluid velocities are decomposed into mean and fluctuating components, $u = \bar{u} + u'$, etc. The quantities $\bar{u}$, $\bar{v}$, and $\bar{w}$ represent the ensemble mean velocities of an infinite number of realizations of the same flow. Correspondingly, we can divide c_i into $\bar{c}_i + c_i'$, where $\bar{c}_i$ is the ensemble mean concentration.

Upon substituting the mean and fluctuating terms into (1) and averaging the resulting equation over the ensemble of flows we obtain the equation governing $\bar{c}_i$. In atmospheric applications, the molecular diffusion term is negligible when compared to that representing advective transport. Thus, neglecting the contribution of molecular diffusion, the equation for $\bar{c}_i$ is

$$\frac{\partial \bar{c}_i}{\partial t} + \bar{u}\frac{\partial \bar{c}_i}{\partial x} + \bar{v}\frac{\partial \bar{c}_i}{\partial y} + \bar{w}\frac{\partial \bar{c}_i}{\partial z} + \frac{\partial}{\partial x}\overline{u'c_i'} + \frac{\partial}{\partial y}\overline{v'c_i'} + \frac{\partial}{\partial z}\overline{w'c_i'}$$

$$= \overline{R_i(c_1, \ldots, c_N, T)} + \bar{S}_i(x,y,z,t) \qquad (2)$$

We note the emergence of the new variables $\overline{u'c_i'}$, $\overline{v'c_i'}$, and $\overline{w'c_i'}$, which represent the fluxes of species i in the three coordinate directions as a result of the velocity fluctuations, u', v' and w'. If species i is involved in second-order chemical reactions then the term $\bar{R}_i$ will also lead to new dependent variables of the form $\overline{c_i'c_j'}$.

Equation (2) is a rigorously valid equation for $\bar{c}_i$ (neglecting, of course, molecular diffusion), and if the variables $\overline{u'c_i'}$, $\overline{v'c_i'}$, $\overline{w'c_i'}$, as well as any of those arising from $\bar{R}_i$, are known as functions of space and time, it can be solved in principle to yield $\bar{c}_i$. Unfortunately, $\overline{u'c_i'}$, etc., cannot be measured at all points in an atmospheric flow, and cannot be predicted exactly because of the closure problem of nonlinear stochastic equations. Thus, we must resort to models for these terms. The model employed in virtually all cases in which atmospheric flows are involved is that based on the concept of eddy diffusivities:

$$\overline{u'c_i'} = -K_H \frac{\partial \bar{c}_i}{\partial x} \qquad \overline{v'c_i'} = -K_H \frac{\partial \bar{c}_i}{\partial y}$$

$$\overline{w'c_i'} = -K_V \frac{\partial \bar{c}_i}{\partial z} \qquad (3)$$

The eddy diffusivities K_H and K_V are postulated to be functions of space and time (and not of $\bar{c}_i$ or any of its gradients). In addition, all models employ the approximation

$$\overline{R_i(c_1,\ldots, c_N,T)} \cong R_i(\bar{c}_1,\ldots, \bar{c}_N,T) \qquad (4)$$

The result of using (3) and (4) in (2) is the so-called *atmospheric diffusion equation,*

$$\frac{\partial \bar{c}_i}{\partial t} + \bar{u}\frac{\partial \bar{c}_i}{\partial x} + \bar{v}\frac{\partial \bar{c}_i}{\partial y} + \bar{w}\frac{\partial \bar{c}_i}{\partial z} = \frac{\partial}{\partial x}\left(K_H \frac{\partial \bar{c}_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \frac{\partial \bar{c}_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_V \frac{\partial \bar{c}_i}{\partial z}\right)$$

$$+ R_i(\bar{c}_1,\ldots, \bar{c}_N,T) + \bar{S}_i(x,y,z,t) \qquad (5)$$

Equation (5) is the fundamental equation upon which most dynamic urban air pollution models are based.

The validity of the atmospheric diffusion equation relates to how closely the predicted mean concentration $\bar{c}_i$ corresponds to the true ensemble mean concentration. If the true ensemble mean velocities and concentrations are known for an atmospheric flow, then it is relatively straightforward to assess the validity of (5) for specified forms of K_H and K_V. Unfortunately, for any atmospheric flow the ensemble mean velocities and concentrations can never be computed since the atmosphere presents only one realization of the flow at any time. (Of course, for a statistically stationary flow, ensemble averages can be replaced by time averages. The atmosphere is, however, seldom in a stationary condition for any appreciable period of time.)

B. FORMULATION OF THE PROBLEM

We denote the measured value of the concentration of pollutant i at monitoring site ℓ at time t_k by $w_{i,\ell}(t_k)$, k = 1,2,... Because there is always some amount of instrument error associated with a measurement, $w_{i,\ell}(t_k)$ is not precisely equal to the *instantaneous* concentration of species i but differs by an error. If it is assumed that this measurement error depends only on the pollutant and not on where or when the measurement is made, then we can write

$$w_{i,\ell}(t_k) = c_i(\underset{\sim}{x}_\ell,t_k) + \varepsilon_i \qquad k = 1,2,\ldots \qquad (6)$$

where $c_i(\underset{\sim}{x}_\ell,t)$ is the instantaneous concentration of i at location $\underset{\sim}{x}_\ell$ [$\underset{\sim}{x} = (x,y,z)$] at time t, and ε_i is the random measurement error for species i. As we noted above, the atmospheric diffusion equation predicts the theoretical ensemble mean concentration $\bar{c}_i(x,t)$. There exists an unknown discrepancy between any instantaneous value and the theoretical mean. In addition, although the atmospheric diffusion equation predicts in principle the mean concentration at all locations, in reality the equation assumes a certain amount of spatial averaging (Lamb and Seinfeld, 1973). In addition, the implementation of the equation requires solution on a finite grid, introducing implicit spatial averages into the computed concentrations. The measurement is, of course, truly a point measurement. Thus, equation (6) becomes

$$w_{i,\ell}(t_k) = \bar{c}_i(\underset{\sim}{x}_\ell,t_k) + \zeta_i(\underset{\sim}{x}_\ell,t_k) + \varepsilon_i \qquad (7)$$

when ζ_i includes all the discrepancies between w_i and $\bar{c}_i$. Because c_i is a random function, ζ_i will itself be a random function.

The random errors in (7) can be combined, so

$$w_{i,\ell}(t_k) = \bar{c}_i(\underset{\sim}{x}_\ell, t_k) + \eta_i(\underset{\sim}{x}_\ell, t_k) \tag{8}$$

where η_i is assumed to have zero mean.

Subsequently we will restrict our attention to inert pollutants or those that decay linearly ($R_i = -k_i\bar{c}_i$). Thus, we need consider only a scalar concentration $\bar{c}(\underset{\sim}{x},t)$ and scalar measurements, $w_\ell(t_k) = \bar{c}(\underset{\sim}{x}_\ell, t_k) + \eta(\underset{\sim}{x}_\ell, t_k)$.

The basic problem of interest is to develop a way of siting new stations in a region with at least some current monitoring stations in which we use the available data and a mathematical air quality model. Our approach is to use the available data and the model to estimate the full spatial and temporal concentration distribution over the region. We consider, therefore, the following problem:

> Estimate the mean concentration $\bar{c}(\underset{\sim}{x},t)$ for $t \geq t_o$ based on the measurements $w_\ell(t_k)$.

In mathematical terms this is a *sequential estimation* or *filtering* problem, i.e., we desire to estimate the state of a dynamic system based on noisy measurements carried out on the system. Filtering theory is a well-developed aspect of mathematical system and control theory. (See, for example, Sage and Melsa, 1971; McGarty, 1974; Jazwinski, 1970.) The air pollution estimation problem has been posed here as a filtering problem, the concentrations being the states. In this case, the system is governed by a set of partial differential equations (5), a so-called *distributed parameter system*. Filtering in distributed parameter systems has received considerable attention. (See, for example, Tzafestas and Nightingale, 1968ab; Tzafestas, 1973; Sakawa, 1972; Hwang et al., 1972; Koda, 1976.) The elements of the distributed parameter filtering theory are given in Appendix A.

The atmospheric diffusion equation (5) is not the "true" equation for the mean concentration $\bar{c}(x,t)$ because of approximations involved in representing turbulent diffusion (assuming that the fluid velocities are exact.) The discrepancy between the true, but unknown, value of $\bar{c}$ and that predicted by (5) can be presented in a simple way by a random error term added to the right hand side (R.H.S.) of (5), $\xi(\underset{\sim}{x},t)$,

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial c}{\partial z} = \frac{\partial}{\partial x}\left(K_H \frac{\partial \bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_V \frac{\partial \bar{c}}{\partial z}\right)$$

$$+ \bar{S}_i(x,y,z,t) + \xi(x,y,z,t) \tag{5'}$$

Thus, we assume that the inaccuracies in the meteorological variables and those arising from inadequate representation of turbulent diffusion can be "lumped" and then quantified as noise in the manner in (5'). Such an additive random error almost certainly does not adequately represent the

discrepancy, although not enough is known about the deviation between the time ensemble mean and that predicted by (5) to attempt to account for the deviation in a more detailed manner. Consequently, we will henceforth assume that a random error $\xi(x,t)$ exists on the R.H.S. of (5) having zero mean and known variance. (The variance of ξ is, of course, not known; it must be estimated based on our judgment as to the essential adequacy of (5) for the given situation.)

The basic filtering procedure is outlined in Figure 1. The basic feature of the filter is that the difference between the measured and estimated concentrations is processed to yield a better estimate of the concentration. In effect, then, the filter is simply a learning algorithm that gets "smarter" as it processes more and more data. The net result is better and better estimates of the concentrations as time progresses.

As illustrated in Figure 1, the "filter" consists of the differential equations for $\hat{c}(\underset{\sim}{x},t)$ and $P(\underset{\sim}{x},\underset{\sim}{y},t)$ that "process" the measurements $w_\ell(t_k)$ to give $\hat{c}(x,t)$. The key problem in the implementation of the distributed parameter filtering theory is the spatial dimensionality of the filter variance P. For a 3-dimensional situation, P is a function of six spatial variables, i.e., $P(x,y,t)$ in vector notation or $P(x,y,z,x',y',z',t)$ in expanded notation. Thus, implementation of the filter requires the numerical solution of the partial differential Riccati equation in six spatial dimensions.

The distributed parameter filtering problem can, in general, be treated in either of two ways with respect to finite-dimensional approximation. The distributed parameter system can be approximated by a lumped-parameter system (i.e., ordinary differential equations) at the very beginning of the problem, and the filtering problem can be solved with respect to the lumped system. This approach can be called "approximation at the beginning." On the other hand, the distributed nature of the problem can be retained throughout the analysis, and only at the point where numerical implementation of the partial differential equations is necessary is a finite-dimensional approximation introduced. This approach can be termed "approximation at the end." From a numerical point of view there does not appear to exist a fundamental advantage for either approach, although approximation at the end does preserve the distributed character of the problem as long as possible. Here we have applied the finite difference approximation at the end.

Clearly, considerations of computation time and storage are paramount. Because of the size of the numerical problem involved in implementing the filter, numerical considerations of accuracy and stability are also important. Covariance square root algorithms are generally more accurate and stable than conventional non-square root algorithms. For this reason we have adopted that approach in solving the filter equations (Appendix C). Technical details of the filter are presented in Appendixes A and B. Table 2 summarizes the general equations of the filter. We note that the filter equation for $\hat{c}$ depends on all the same variables and phenomena as the original atmospheric diffusion equation. On the other hand, the variance equation for P is independent of the source emissions.

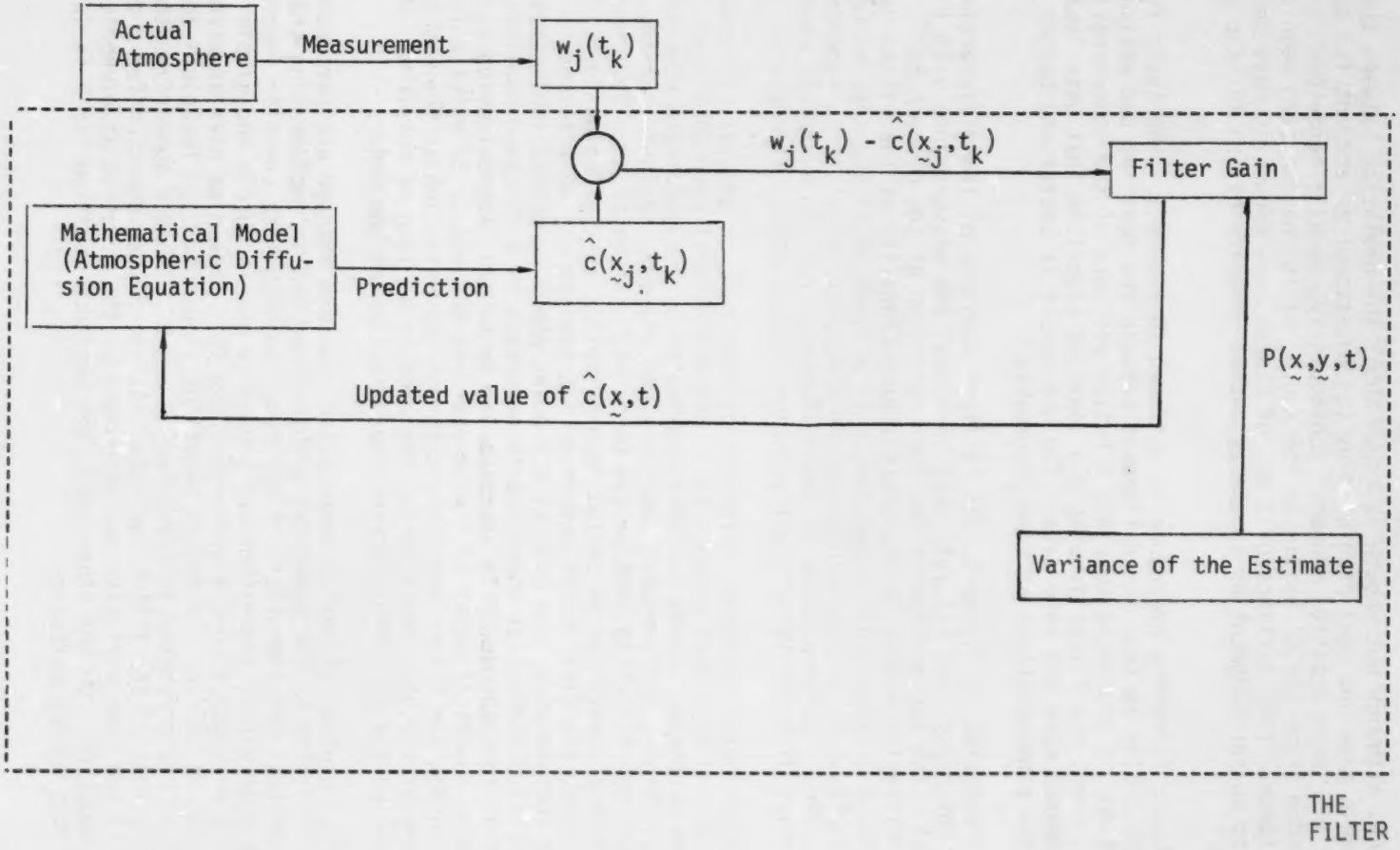


Figure 1. Basic filtering procedure for estimating air pollutant concentrations

TABLE 2. OPTIMAL DISTRIBUTED-PARAMETER FILTER

Diffusion Process	$\frac{\partial c(\underset{\sim}{x},t)}{\partial t} = L_x c(\underset{\sim}{x},t) + \xi(\underset{\sim}{x},t)$,	$\underset{\sim}{x} \in \Omega$
	$L_b\, c(\underset{\sim}{x},t) = \phi(\underset{\sim}{x},t)$,	$\underset{\sim}{x} \in \partial\Omega$
Measurement	$w_\ell(t_k) = c(\underset{\sim}{x}_\ell,t_k) + \eta_\ell(t_k)$,	$\ell = 1,2,\ldots, M;\ k = 1,2,\ldots$
	Time Update Filtering Equations $(t_k^+ \le t \le t_{k+1}^-)$	
Estimate	$\frac{\partial \hat{c}(\underset{\sim}{x},t)}{\partial t} = L_x \hat{c}(\underset{\sim}{x},t)$,	$\underset{\sim}{x} \in \Omega$
	$L_b \hat{c}(\underset{\sim}{x},t) = \phi(\underset{\sim}{x},t)$,	$\underset{\sim}{x} \in \partial\Omega$
Variance	$\frac{\partial P(\underset{\sim}{x},\underset{\sim}{y},t)}{\partial t} = L_x P(\underset{\sim}{x},\underset{\sim}{y},t) + P(\underset{\sim}{x},\underset{\sim}{y},t)L_y' + Q(\underset{\sim}{x},\underset{\sim}{y},t)$,	$\underset{\sim}{x},\ \underset{\sim}{y} \in \Omega$
	$L_b P(\underset{\sim}{x},\underset{\sim}{y},t) = 0$,	$\underset{\sim}{x} \in \partial\Omega$
	$P(\underset{\sim}{x},\underset{\sim}{y},t)L_b' = 0$,	$\underset{\sim}{y} \in \partial\Omega$
	Measurement Update Filtering Equations $(t = t_k)$	
Estimate	$\hat{c}(\underset{\sim}{x},t_k^+) = \hat{c}(\underset{\sim}{x},t_k^-) + \sum_{i=1}^{M}\sum_{j=1}^{M} P(\underset{\sim}{x},\underset{\sim}{s}_i,t_k^-)[\Lambda^{-1}(t_k)]_{ij}[w_j(t_k) - \hat{c}(\underset{\sim}{s}_j,t_k^-)]$	
Variance	$P(\underset{\sim}{x},\underset{\sim}{y},t_k^+) = P(\underset{\sim}{x},\underset{\sim}{y},t_k^-) - \sum_{i=1}^{M}\sum_{j=1}^{M} P(\underset{\sim}{x},\underset{\sim}{s}_i,t_k^-)[\Lambda^{-1}(t_k)]_{ij} P(\underset{\sim}{s}_j,\underset{\sim}{y},t_k^-)$	
	$[\Lambda(t_k)]_{ij} = P(\underset{\sim}{s}_i,\underset{\sim}{s}_j,t_k^-) + R_{ij}(t_k)$	

Table 2 summarizes the filter in general form, based on the development in Appendix A. In the next section we develop a basic regional air pollution model based on a 3-dimensional form of the atmospheric diffusion equation and present the specific equations of the filter corresponding to that model. A computer code has been developed that solves the atmospheric diffusion equation together with the equations for $\hat{c}(x,y,z,t)$ and $P(x,y,z,x',y',z',t)$. The code is detailed in Appendix E. The code is applicable to all problems that can be posed as obeying the general model of Section III.C. For the purposes of illustrating the performance of the filter we choose in Section III.C a set of specific parameter values. Section III.D is devoted to the results of applying the general code to the specific situation defined in Section III.C.

C. BASIC REGIONAL MODEL FOR APPLICATION OF FILTERING THEORY

We adopt the following assumptions in regard to the basic atmospheric diffusion equation (5):

1) The surface of the ground is flat so that atmospheric motion is 2-dimensional, and vertical wind velocity components can be neglected.

2) Turbulent diffusion in the horizontal direction is negligible as compared with horizontal advection.

3) The location of sources is defined through a boundary condition in the form of surface flux.

4) There is a temperature inversion layer at a given elevation.

Using the same notation as in the previous section, the diffusion equation governing a single species in the atmosphere, under these assumptions is (dropping the overbar for convenience)

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} = \frac{\partial}{\partial z}\left\{K_V \frac{\partial c}{\partial z}\right\} + \xi(x,y,z,t) \tag{9}$$

where ξ is an artificial random forcing term to account for discrepancies between c as predicted by (5) and the true (but unknown) ensemble mean concentration. It is unlikely that an additive random term properly accounts for this modeling error, although without further information we resort to this assumption. Further, we shall assume that ξ is well-represented by a distributed white Gaussian process with the following properties:

$$E\{\xi(x,y,z,t)\} = 0 \tag{10}$$

$$E\{\xi(x,y,z,t)\xi(x',y',z',\tau)\} = Q(x,y,z,x',y',z',t)\delta(t-\tau)$$

where the variance function Q is positive semi-definite and symmetric with respect to the spatial coordinates (x,y,z) and (x',y',z').

The vertical boundary conditions used are

$$- K_{vo} \frac{\partial c}{\partial z} = S(x,y,t) \qquad \text{at } z = 0$$

$$\frac{\partial c}{\partial z} = 0 \qquad \text{at } z = Z_{max} \tag{11}$$

where K_{vo} is the eddy diffusivity at ground level and $S(x,y,t)$ is the surface flux and is a specified deterministic function. Other boundary conditions are given at the upstream boundaries:

$$c(0,y,z,t) = c_b$$

$$c(x,0,z,t) = c_b \tag{12}$$

where c_b can be a function of time. It can be assumed that the exact value of c_b is not given as a priori information.

The initial conditions necessary for an unsteady state model (9) are now known precisely, and only the estimated mean concentration

$$E\{c(x,y,z,0)\} = \hat{c}_o(x,y,z) \tag{13}$$

and its variance

$$E\{[c(x,y,z,0) - \hat{c}_o(x,y,z)][c(x',y',z',0) - \hat{c}_o(x',y',z')]\}$$

$$= P_o(x,y,z,x',y',z') \tag{14}$$

are assumed to be known.

The measurement data are usually available at discrete times, t_k, $k = 1, 2, \ldots$, only at discrete locations. Hence the measurement process is represented as

$$w_\ell(t_k) = c(x_\ell,y_\ell,z_\ell,t_k) + \eta_\ell(t_k) , \qquad \ell = 1,2,\ldots, M \tag{15}$$

where $\eta_\ell(t_k)$ is the error associated with a measurement $w_\ell(t_k)$. We shall assume that $\eta_\ell(t_k)$ is a white Gaussian noise sequence with properties:

$$E\{\eta_i(t_n)\} = 0$$

$$E\{\eta_i(t_n)\eta_j(t_m)\} = R_{ij}(t_n)\delta_{mn} \tag{16}$$

where $R_{ij}(t_n)$ is a positive variance.

We shall assume that the random variables $\xi(x,y,z,t)$, $c(x,y,z,0)$, and $\eta_\ell(t_k)$ are mutually statistically independent. It is then necessary to specify the variances $Q(x,y,z,x',y',z',t)$ and $R_{ij}(t_k)$. The proper specification of these functions is a major problem in the ultimate implementation of the theory. For example, the form of $R_{ij}(t_k)$ will depend on how the discrepancies between data and prediction are expected to vary with location. Such

information can be obtained through a statistical analysis of past modeling studies comparing predictions to data. At present, we do not assume that correlations exist between the errors in measurements and the modeling errors of different locations. Hence we can write

$$Q(x,y,z,x',y',z',t) = Q(x,y,z,t)\delta(x'-x)\delta(y'-y)\delta(z'-z) \tag{17}$$

$$R_{ij}(t_k) = R_i(t_k)\delta_{ij} \tag{18}$$

Thus, we have constructed a simple, but sufficiently general, model of air pollution for application of the filtering theory.

For a convenience, a dimensionless form of the model equations is utilized. Let C_r, T_r, L_r, U_r, K_r, and S_r denote arbitrary reference values for concentration, time, spatial length, wind speed, eddy diffusivity, and surface flux, respectively. Then, using these reference values, the dimensionless form of (9) becomes

$$\frac{\partial c^*}{\partial t^*} = -\frac{T_r U_r}{L_r}\left(u^*\frac{\partial c^*}{\partial x^*} + v^*\frac{\partial c^*}{\partial y^*}\right) + \frac{T_r K_r}{L_r^2}\frac{\partial}{\partial z^*}\left(K_v^*\frac{\partial c^*}{\partial z^*}\right) + \xi^* \tag{19}$$

where the superscript * denotes a dimensionless quantity. In a similar manner, other equations above can be easily transformed to a dimensionless form.

The following set of reference values is specified to unity throughout the simulation:

$$C_r = 1 \quad [\text{ppm}]$$

$$K_r = 1 \quad [m^2/s]$$

$$U_r = 1 \quad [m/s]$$

Using these special reference values, the computer input and output variables, i.e., the dimensionless values K_v^*, u^*, v^*, and c^*, correspond to their actual physical values but are dimensionless. Other reference values will be determined based on the grid square size employed in the discretization.†

In the process of discretization necessary to implement the filter, we have used finite difference methods. The primary source of errors associated with the finite difference approximation arises in the discretization of the spatial coordinates. Although the analysis shows that the higher order truncation terms always vanish when higher order finite difference schemes are used, this phenomenon does not necessarily imply that these schemes are more suitable. A notorious example can be found in airshed modeling: near localized sources, higher order schemes predict negative concentrations, whereas simple first-order schemes do not.

† Process by which a continuous spatial domain is represented by an array of cells for the purposes of numerical computation.

In order to ascertain numerical stability and accuracy we have applied the time-splitting technique to the finite difference implementation of (19). (For details see Appendix B.) In this time-splitting concept, the original advection-diffusion equation (19) is decomposed into the 2-dimensional "advection part," and into the 1-dimensional "diffusion part."

(a) Advection part:

$$\frac{\partial c^*}{\partial t^*} = - \frac{T_r U_r}{L_r} \left(u^* \frac{\partial c^*}{\partial x^*} + v^* \frac{\partial c^*}{\partial y^*} \right) \tag{20}$$

(b) Diffusion part:

$$\frac{\partial c^*}{\partial t^*} = \frac{T_r K_r}{L_r^2} \frac{\partial}{\partial z^*} \left\{ K_v^* \frac{\partial c^*}{\partial z^*} \right\} \tag{21}$$

Then stable finite difference methods suitable for (20) and (21) are applied independently. We have applied Fromm's (1968) second-order, zero-average, phase error method to the advection part (20). The standard Crank-Nicolson second-order method has been applied to the diffusion part (21). These second-order schemes improved the numerical accuracy and stability and did not lead to negative concentrations.

The stability of Fromm's second-order, zero-average phase error method can be easily evaluated for the advection part (20). The evaluation of the artificial (or pseudo) diffusion term associated with the method leads to the Courant condition for stability:

$$\frac{T_r U_r}{L_r} \quad (\alpha + \beta) < 1 \tag{22}$$

where α and β denote the Courant numbers defined as

$$\alpha = \frac{u^* \Delta t^*}{\Delta x^*}$$

$$\beta = \frac{v^* \Delta t^*}{\Delta y^*} \tag{23}$$

where Δx^*, Δy^*, and Δt^* are the dimensionless mesh spacing in the x, y, and t coordinate directions, respectively

Using the Courant condition (22), we can generate the following table for the various combinations of L_r and T_r.

TABLE 3. STABILITY CONDITIONS

T_r[sec]	L_r[m]	$T_r U_r/L_r$	$T_r K_r/L_r^2$	Stability Condition
1	100	0.01	0.0001	$\Delta x^* \geq 0.02(u^*)_{max}\ \Delta t^*$
				$(\Delta y^* \geq 0.02(v^*)_{max}\Delta t^*)$
30	1000	0.03	0.00003	$\Delta x^* \geq 0.06(u^*)_{max}\Delta t^*$
60	1000	0.06	0.00006	$\Delta x^* \geq 0.12(u^*)_{max}\Delta t^*$

We note that the stability of the method depends on the dimensionless wind velocity components $(u^*)_{max}$ and $(v^*)_{max}$, as well as on the spacing Δx^*, Δy^*, and Δt^*. The spacing Δx^*, Δy^*, and Δt^* are usually determined by the computer memory storage and computation time requirements. For most air pollution situations, both u* and v* range in value between 0 and 10 on the dimensionless scale. Consideration of actual air pollution applications leads to the following reference values for T_r and L_r:

$$T_r = 60 \text{ [sec]} = 1 \text{ [min]}$$

$$L_r = 1000 \text{ [m]} = 1 \text{ [km]}$$

1. Scale Transformation in Vertical Direction

In the estimation problem, we are mainly concerned with the estimation of concentrations near the ground level. Most of the stations in a given area provide measurement readings representative of the average grid-square concentrations at the height of receptor location. Measurements reported by the monitoring stations then are used as inputs to the filter to compute estimates near the ground level averaged over the square grid area. Hence, it may be very useful if a filter can quite effectively calculate the estimates representative of the average grid-square concentrations at the level of measurement height. For this reason, a fairly detailed finite difference representation is performed for the vertical diffusion part (21).

Consider the following scale transformation in the vertical direction,

$$z^* = h(\exp z - 1)/(\exp \Delta z - 1)$$
$$z_k = (k - 1)\Delta z \qquad (24)$$

where z is the transformed dimensionless value of z*, Δz is the spacing in this new coordinate system, and h is the effective height of measurement. The definition of the effective height of measurement is apparent from (24).

Using this scale transformation in the finite difference implementation of the diffusion part (21), we can calculate the concentrations near the effective height of measurement more accurately than by using a standard equally-space, finite-difference representation. This transformation is illustrated in Figure 2 for $\Delta z = 0.5$ and $h = 15$.

(a) Advection part:

$$\frac{\partial c}{\partial t} = - 0.06 \left(u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} \right) \tag{25}$$

(b) Diffusion part:

$$\frac{\partial c}{\partial t} = 0.00006 \frac{(\exp\Delta z - 1)^2}{h^2 \exp z} \frac{\partial}{\partial z} \left\{ \frac{K_v}{\exp z} \frac{\partial c}{\partial z} \right\} \tag{26}$$

where, for the convenience of notation, we have dropped the superscript *. Thus, we now apply the finite difference methods to (25) and (26).

2. Mesh Parameters

The mesh used in the computation is shown in Figure 3. We have selected the following mesh parameters:

$\Delta t = 1.5$
$\Delta x = \Delta y = 2$
$\Delta z = 0.5$
$h = 15/1000$
$N_x = N_y = 13$
$N_z = 6$

where N_x, N_y, and N_z are mesh numbers along x-, y-, and z-direction, respectively. This mesh system, which is used for the computation of the estimated concentrations, is a refinement of the mesh that is used for the computation of the variances. The coarse mesh which is indicated by the bold line in Figure 3 is used for the computation of the filter variances. The mesh parameters used in the computation of the filter variances are:

$\Delta t = 1.5$
$\Delta x = \Delta y = 4$
$\Delta z = 0.5$
$h = 15/1000$
$N_x = N_y = 7$
$N_z = 6$

These mesh parameters are determined from the considerations of computer memory storage and computation time requirements. Using these mesh systems, the computer storage required for the filter is the order of one megabyte

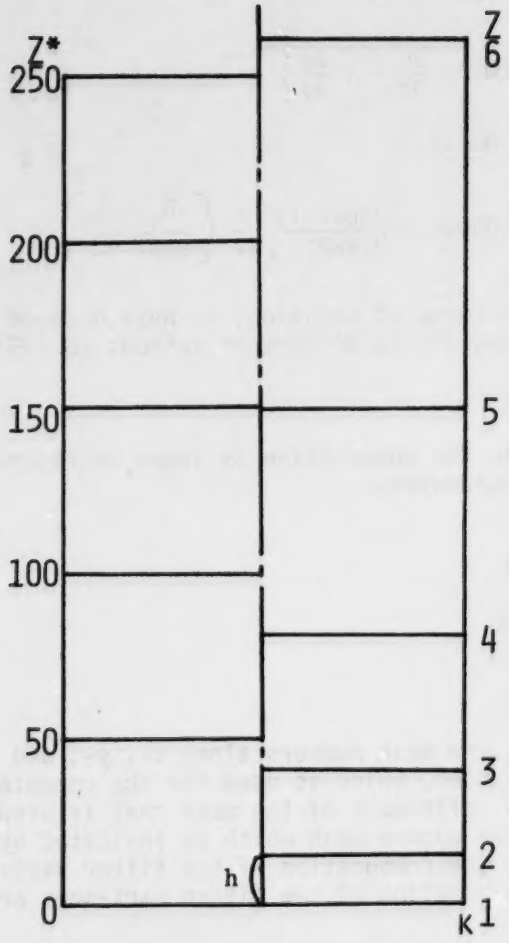
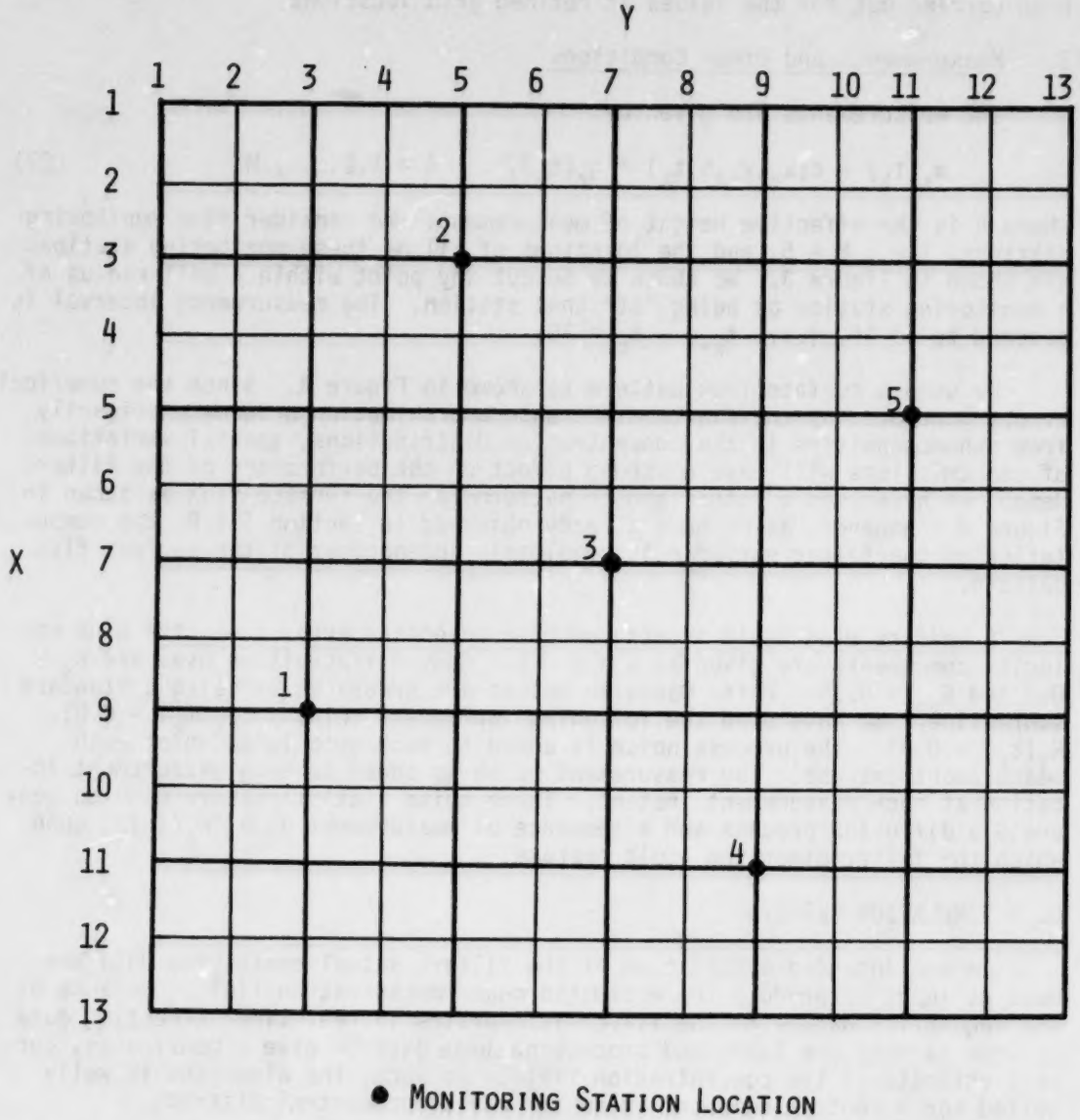


Figure 2. Scale transformation in vertical direction



● MONITORING STATION LOCATION

Figure 3. Basic grid system for computation

or more for the IBM 370/158 system. In the measurement update computation of the filter state, intermesh (spatial) interpolation calculations have been carried out for the values at refined grid locations.

3. Measurements and Other Conditions

The measurements are given by

$$w_\ell(t_k) = c(x_\ell, y_\ell, h, t_k) + \eta_\ell(t_k), \qquad \ell = 1,2,\ldots, M \tag{27}$$

where h is the effective height of measurement. We consider five monitoring stations, i.e., M = 5, and the locations of all of these monitoring stations are shown in Figure 3. We chose to accept any point within a unit radius of a monitoring station as being "at" that station. The measurement interval is assumed to be 15, i.e., $t_{k+1} - t_k = 15$.

We used a surface flux pattern as shown in Figure 4. Since the numerical errors generated by the finite difference approximation originate primarily from inhomogeneities in the concentration distributions, spatial variations of the emissions will have a strong effect on the performance of the filter. Hence, we have used a rather smooth pattern for the surface flux as shown in Figure 4. However, as we have already observed in Section III.B, the computation of the filter variance is completely independent of the surface flux pattern.

A uniform wind field is assumed over an entire area, i.e., the wind velocity components are given as u = v = 2. Eddy diffusivities used are K_y = 0.7 and K_{yo} = 0.35. White Gaussian noises are generated by using a standard subroutine. We have used the following variances: $Q(x_i, y_i, z_i, t_k) = 0.01$, $R_i(t_k) = 0.01$. The process noise is added to each grid location at each measurement instant. The measurement noise is added to each measurement location at each measurement instant. These noise statistics were used to generate a diffusion process and a sequence of measurement data $\{w_\ell(t_k)\}$, upon which the filter algorithm would operate.

D. SIMULATION RESULTS

In the intended application of the filter, actual monitoring data are used as input to produce the estimated mean concentration field. Because of the sequential nature of the filter it operates in real time, accepting data as soon as they are taken and processing those data to give a continuous, current estimate of the concentration field. As such, the algorithm is well-suited for a central computer in an air pollution control district.

In the present study the monitoring data were simulated numerically by integrating the model developed in Section III.C and artificially corrupting the "exact" concentrations with random dynamic, $\xi(\underset{\sim}{x},t)$, and measurement, $\eta(\underset{\sim}{x},t)$, errors to produce the "data," $w_j(t_k)$. The value of such a numerical experiment is that the true concentrations are known, and, consequently, the performance of the filter can be evaluated quantitatively under a variety of circumstances. Two basic situations were studied:

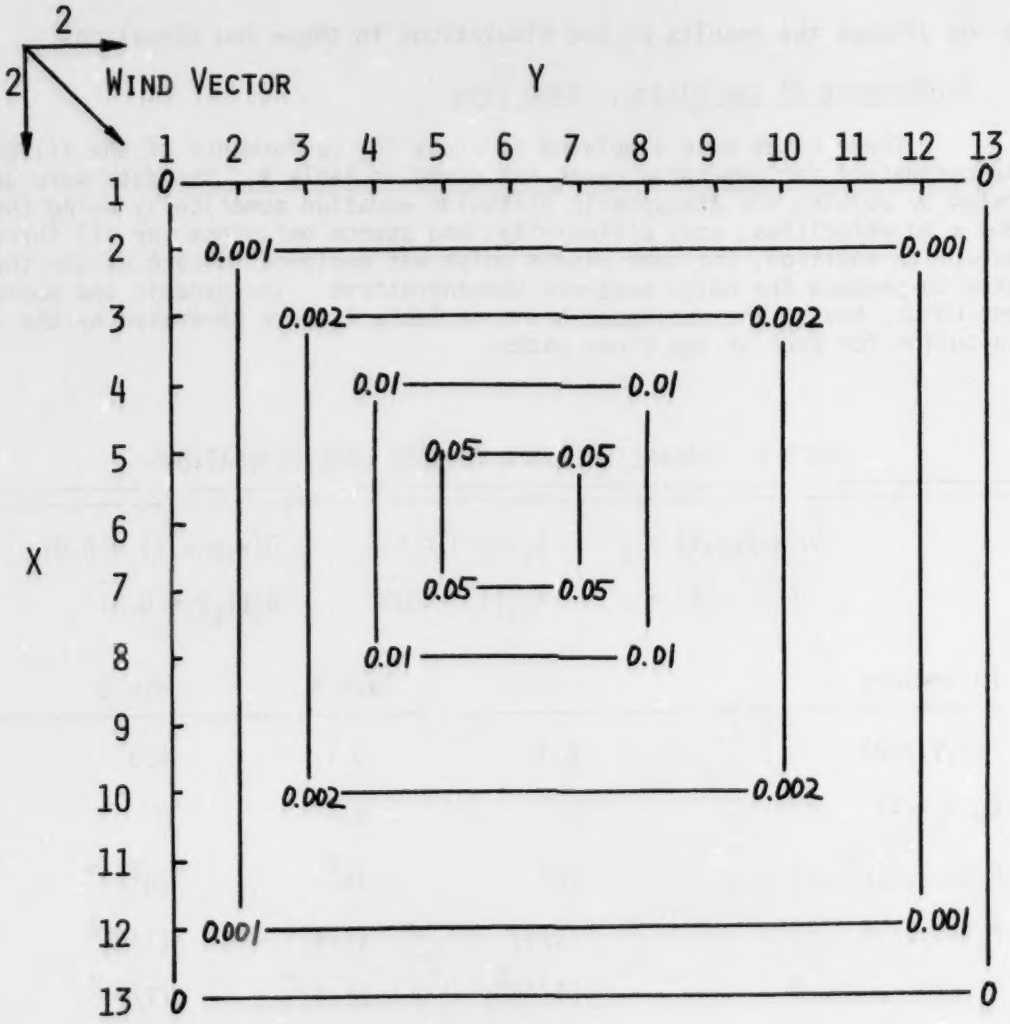


Figure 4. Spatial distribution of pollutant surface flux

1. The performance of the filter was studied as a function of some of the basic parameters of the problem for the base case described in Section III.C, namely five monitoring stations in the hypothetical region of Figure 3.

2. The performance of the filter was studied as a function of the number of monitoring stations.

We now discuss the results of the simulations in these two situations.

1. Performance of the Filter. Base Case

Three cases were simulated to study the performance of the filter. The parameters for the three cases are given in Table 4. The data were generated by solving the atmospheric diffusion equation numerically using the same wind velocities, eddy diffusivity, and source emissions for all three cases. In addition, the same random noise was employed in each of the three cases to produce the noisy measured concentrations. The dynamic and measurement noise, having the variances given in Table 4, were generated by the same subroutine for each of the three cases.

TABLE 4. PARAMETERS USED IN BASE CASE SIMULATIONS

$u(x,y,z,t) = 2$ $\quad K_V(z,t) = 0.7$ $\quad Q(x,y,z,t) = 0.01$

$v(x,y,z,t) = 2$ $\quad K_{Vo}(t) = 0.35$ $\quad R_i(t_k) = 0.01$

Parameters	Case A	Case B	Case C
$c(x,y,z,0)$	0.1	0.1	0.3
$\hat{c}_o(x,y,z)$	0	0	0
$P_o(x,y,z,x,y,z)$	10^2	10^4	10^2
$P_o(0,y,z,0,y,z)$	$(1/4)^2$	$(1/4)^2$	$(1/4)^2$
$P_o(x,0,z,x,0,z)$	$(1/4)^2$	$(1/4)^2$	$(1/4)^2$
$P_o(x,y,z,x',y',z')$ $x' \neq x, y' \neq y, z' \neq z$	0	0	0

Numerical ill-conditioning of the filter often results when there are large initial uncertainties and relatively small noise variances. Thus, we specifically considered such a situation to test the convergence of the filter to the actual concentrations. The noise variances, $Q(x,y,z,t)$ and $R_i(t_k)$ were chosen to be relatively small (0.01) so that measurements at low concentration were the same order as the errors. A large initial uncertainty was assumed in case B, $P_0(x,y,z,x,y,z) = 10^4$, whereas relatively small initial uncertainties were chosen for cases A and C, $P_0(x,y,z,x,y,z) = 10^2$. Initial uncertainties at the upstream boundaries are small, $(1/4)^2$, because we have assumed that these boundary concentrations are relatively well known. The true initial conditions are different in cases A and C, whereas the initial estimates are taken to be the same.

Let us consider first the behavior of the variance $P(x,y,z,x',y',z',t)$ for the simulated cases. (Note that P is independent of the actual data and depends only on P_0, Q and R.) Figures 5† and 6 show $P(x_i,y_i,h,x_i,y_i,h,t_k)$ for cases A and B of Table 3 at each of the five measurement locations. These values represent the variance of the estimate error at height h,

$$P(x_i,y_i,h,x_i,y_i,h,t_k) = E\{[c(x_i,y_i,h,t_k) - \hat{c}(x_i,y_i,h,t_k)]^2\}$$

Figures 7 and 8 show $P(x,y,h,x,y,h,t_k)$. The algorithm is seen to guarantee nonnegativity of the computed variances. Moreover, the variances show the same general trend in cases A and B. The numerical stability of the square root algorithm is evidenced by the lack of sensitivity of P to the choice of a priori variance for the low noise level cases.

The estimated concentrations at each of the five measurement locations are compared with the true and measured concentrations in Figures 9 and 10 for cases A and C, respectively. In both cases the estimates display the same general agreement with the true concentrations, and the estimates are, as expected, closer to the true concentrations than are the measurements. The true and estimated concentration distributions are compared in Figure 11 for case A. Similar distributions are shown in Figure 12 for case C. Simulation and accuracy results for case C were consistently similar to those for case A.

Estimation error variances are shown in Figures 13 and 14 for cases A and C, respectively. The actual error variances are considerably smaller than those predicted by the filter shown in Figures 5 and 6. Thus, good filter performance is demonstrated in situations with relatively low levels of dynamic and measurement noise, situations often prone to numerical errors.

The estimated concentration is compared with the true concentration for case A in Figure 15. The estimated concentration field tends to be smoother than the actual field. This behavior reflects the smoothing aspects of the filter.

The computer storage and time requirements for the simulations of Table 3 were (IBM 370/158)

†In this and subsequent figures, numbers on the curves refer to the monitoring locations in Figure 2.

Core memory	1100 K bytes
Computation time (CPU)	78.5 min

2. Performance of the Filter. Effect of Number of Measurement Locations

Simulation studies were performed to evaluate the effects of the number of measurement locations. Case A of the former section was selected as the base case. The five measurement locations shown in Figure 3 represent the potential monitoring sites. Three measurement situations have been considered. The conditions for the three cases are given in Table 5. Other parameters of the simulation are the same as those given in Table 4 for case A. Monitoring station 3, which is located at the center of the region, is used in all three cases. The three monitoring stations used in Case II were chosen arbitrarily.

The estimation results are compared at each of the potential monitoring sites in Figure 16. The most surprising result of this simulation is the fact that the filtering algorithm is able to generate meaningful, but not accurate, state estimates even in case I in which only one measurement station exists. The results of case I at the potential monitoring site 4 are not acceptable since the concentrations are poorly estimated at the end of the simulation. The results of cases II and III are acceptable, however.

The calculated filter variances and the actual estimation error variances are shown in Figure 17 as a function of the number of measurements. In Figure 17, the plotted values represent the calculated filter variance

TABLE 5. MEASUREMENT CONDITIONS

Base Case		Case A		
Measurement Situations		Case I	Case II	Case III
Number of Measurements		1	3	5
Monitoring Station (Figure 3)	1	-	0	0
	2	-	0	0
	3	0	0	0
	4	-	-	0
	5	-	-	0

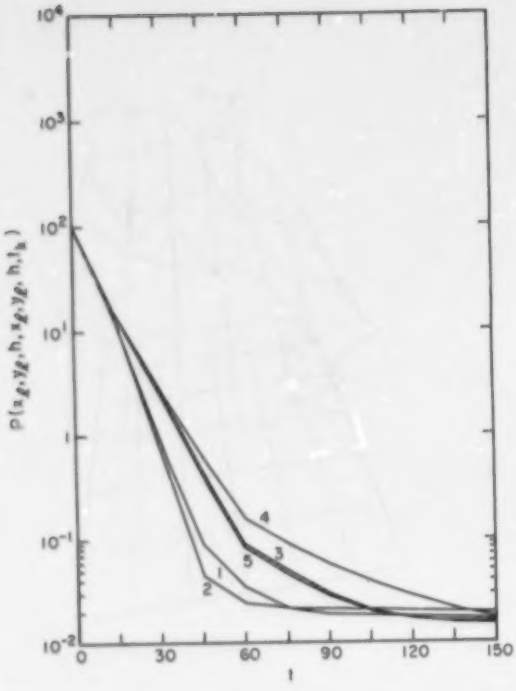


Figure 5. Computed filter variance, case A.

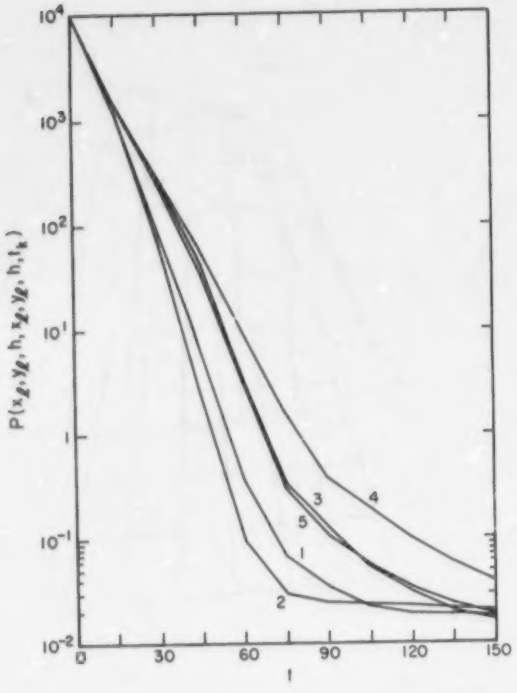


Figure 6. Computed filter variance, case B.

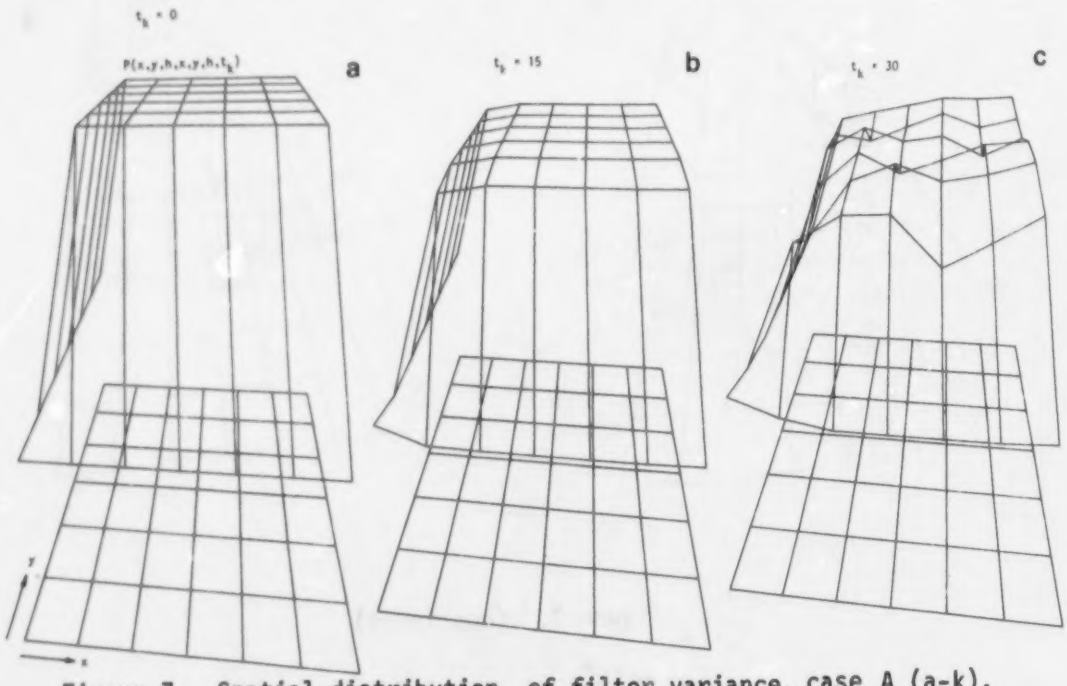


Figure 7. Spatial distribution of filter variance, case A (a-k).

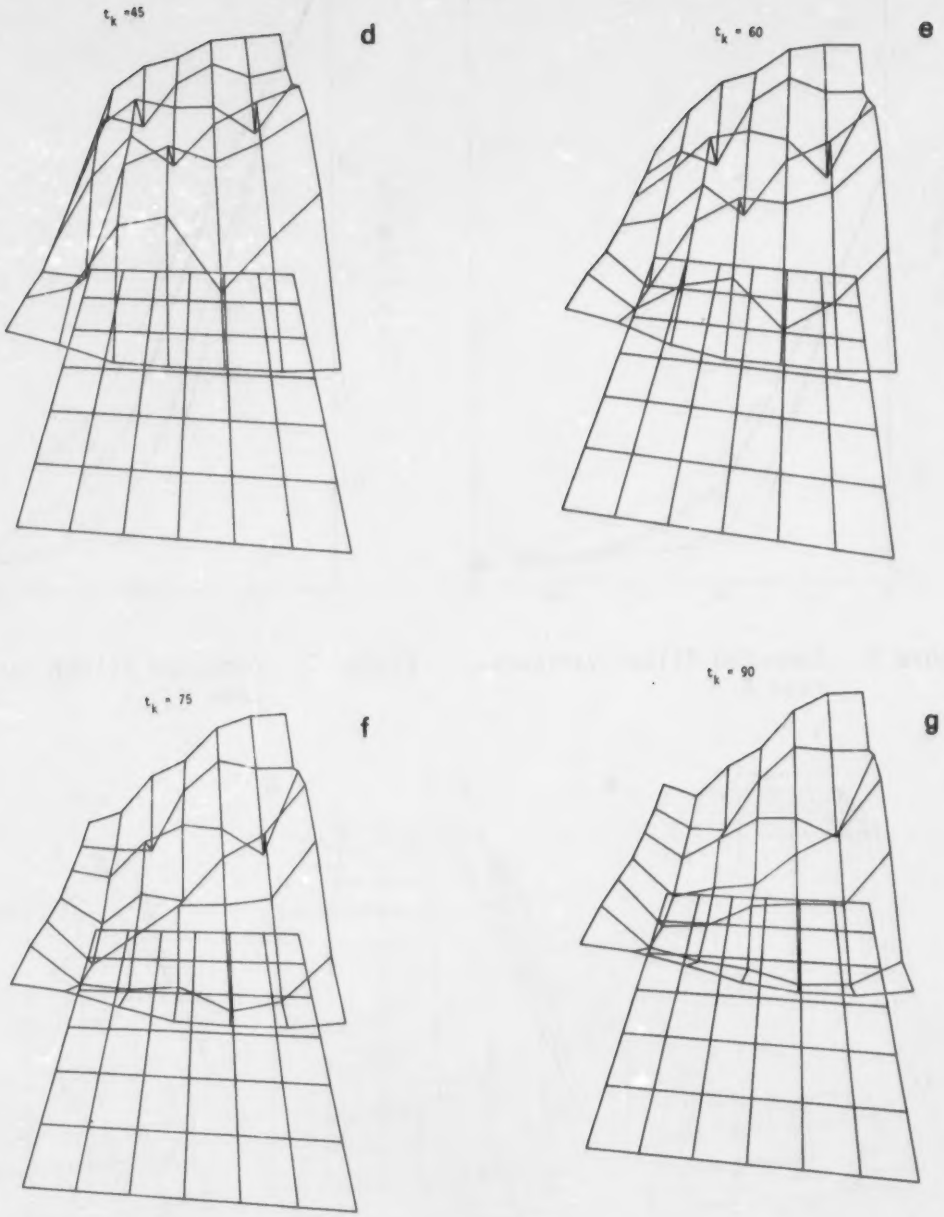


Figure 7. (continued)

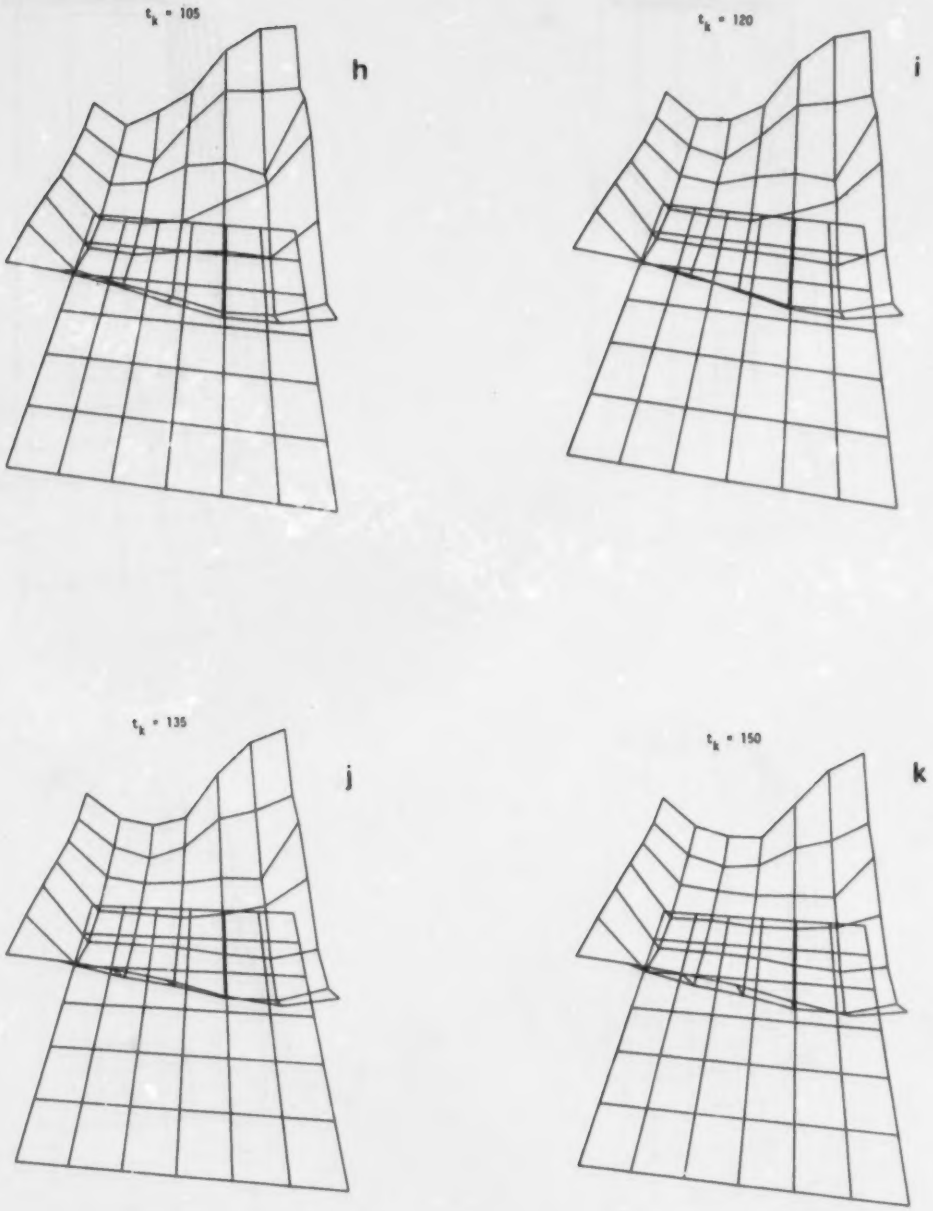


Figure 7. (continued)

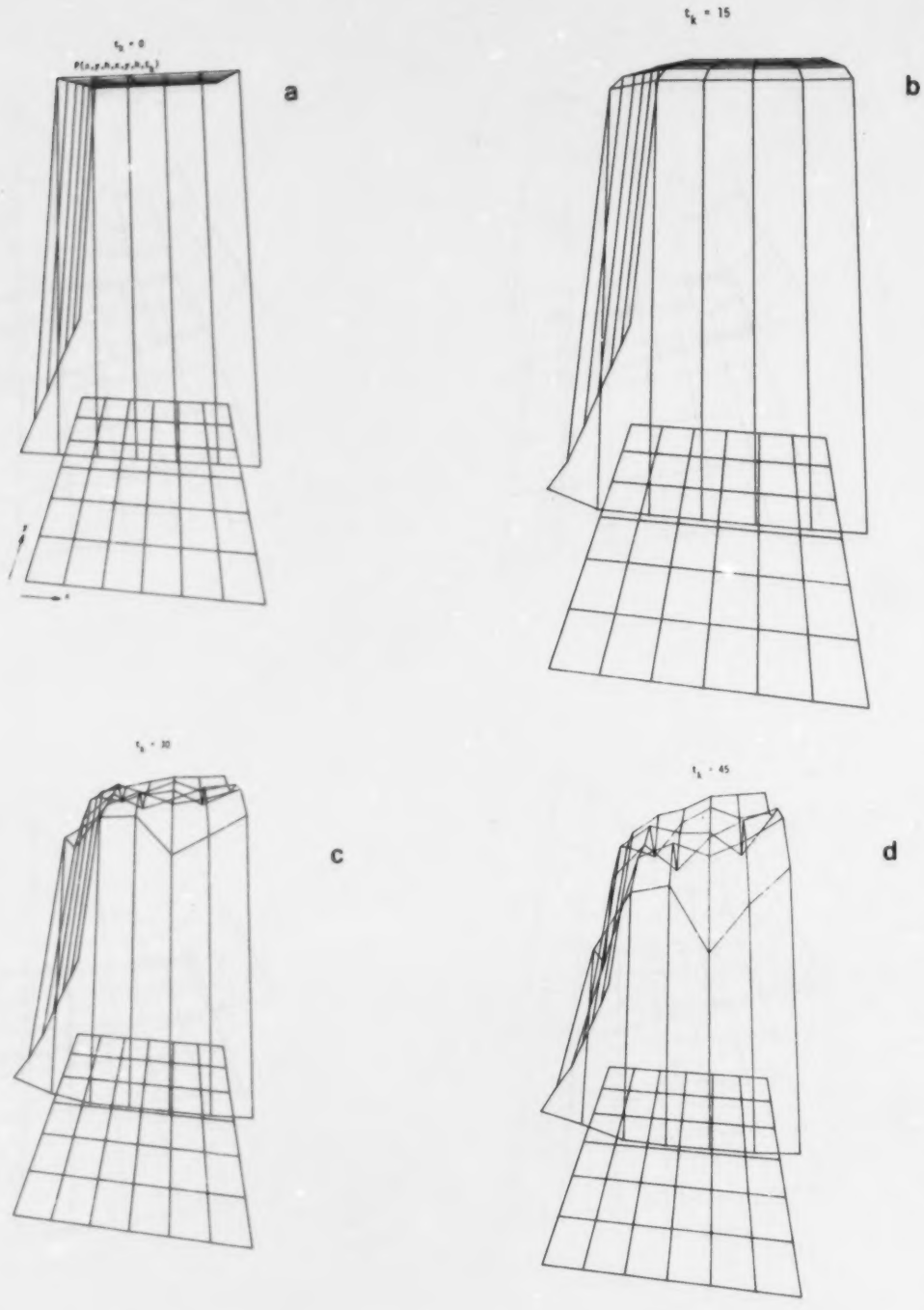


Figure 8. Spatial distribution of filter variance, case B (a-k).

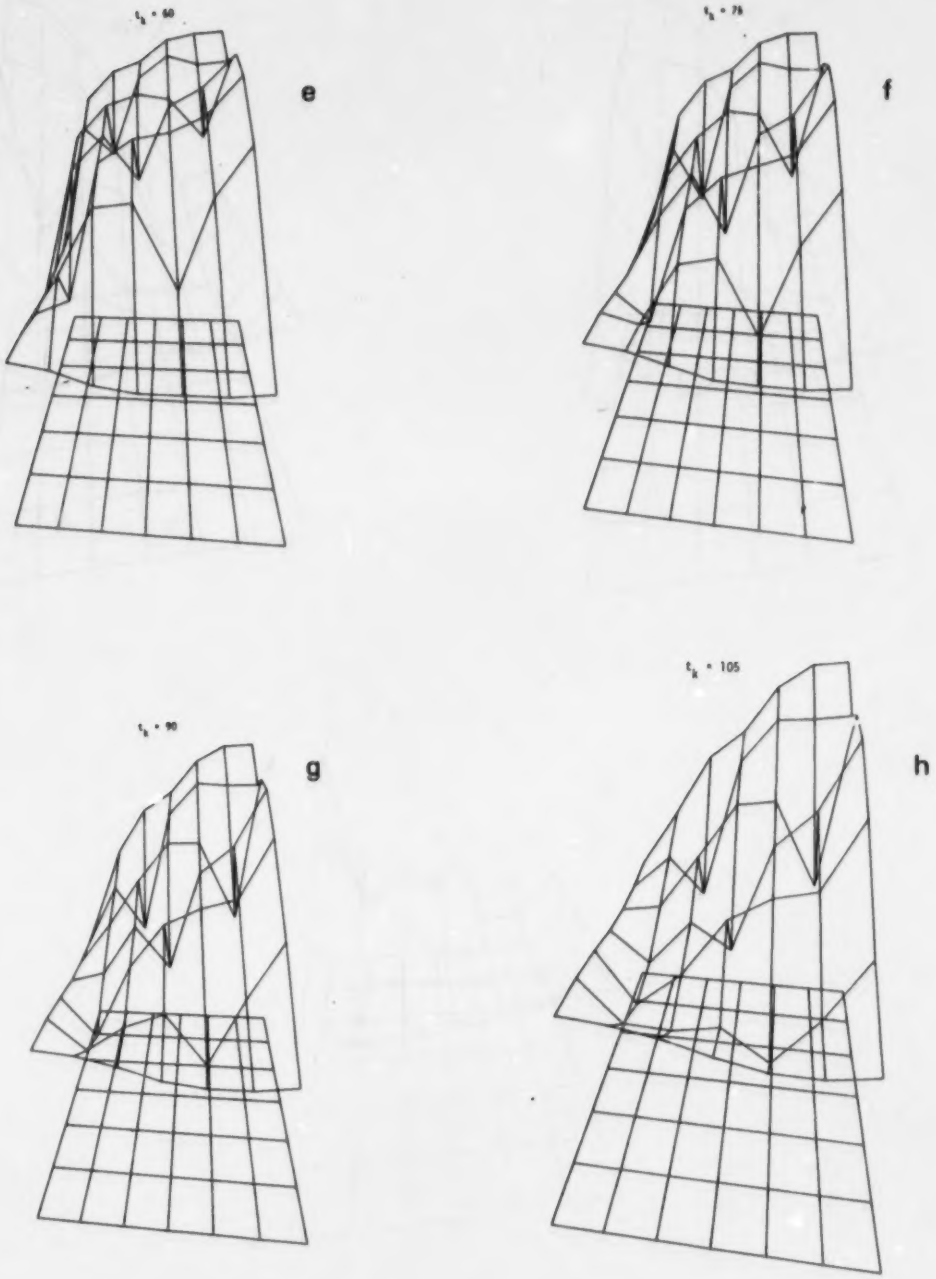


Figure 8. (continued)

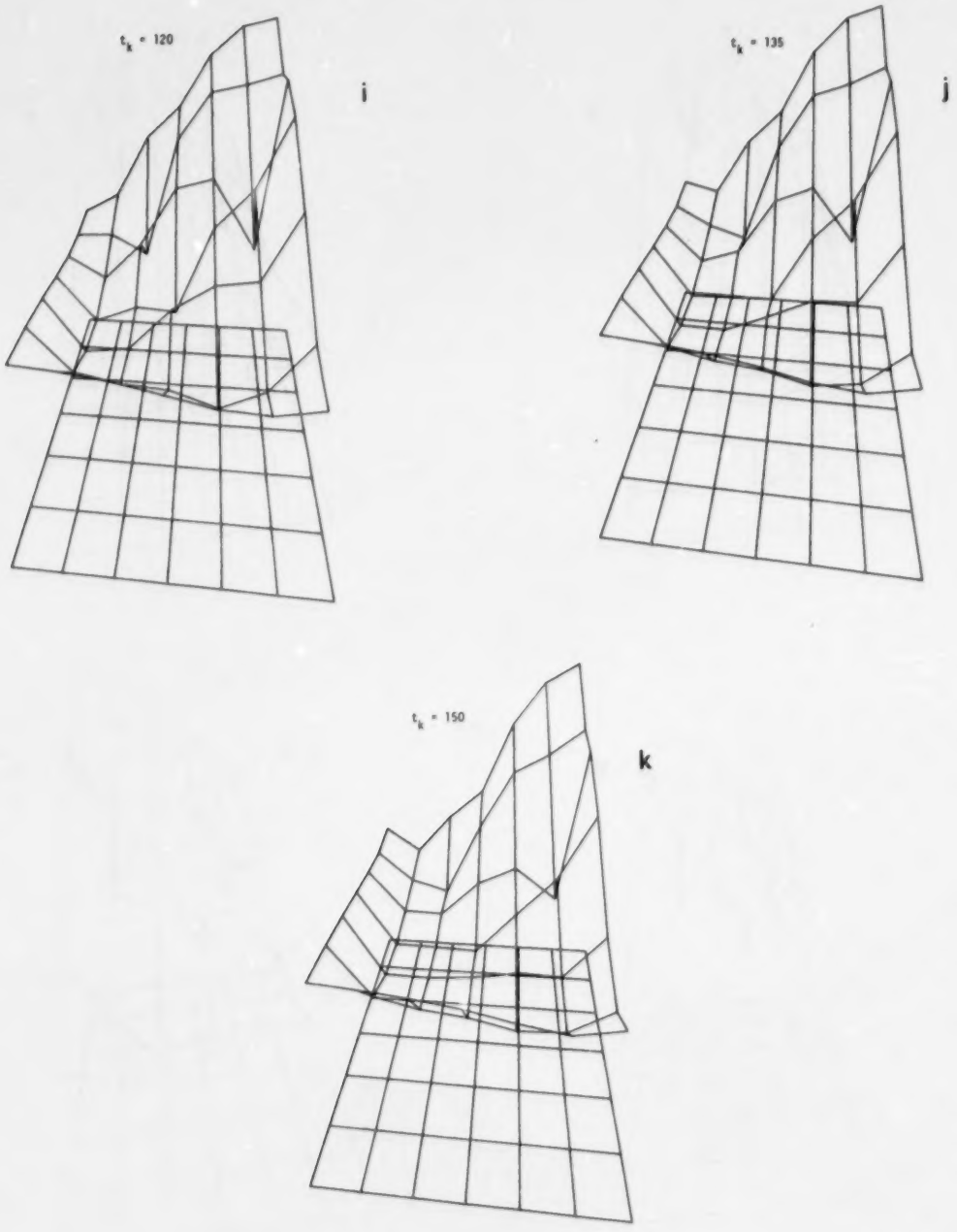


Figure 8. (continued)

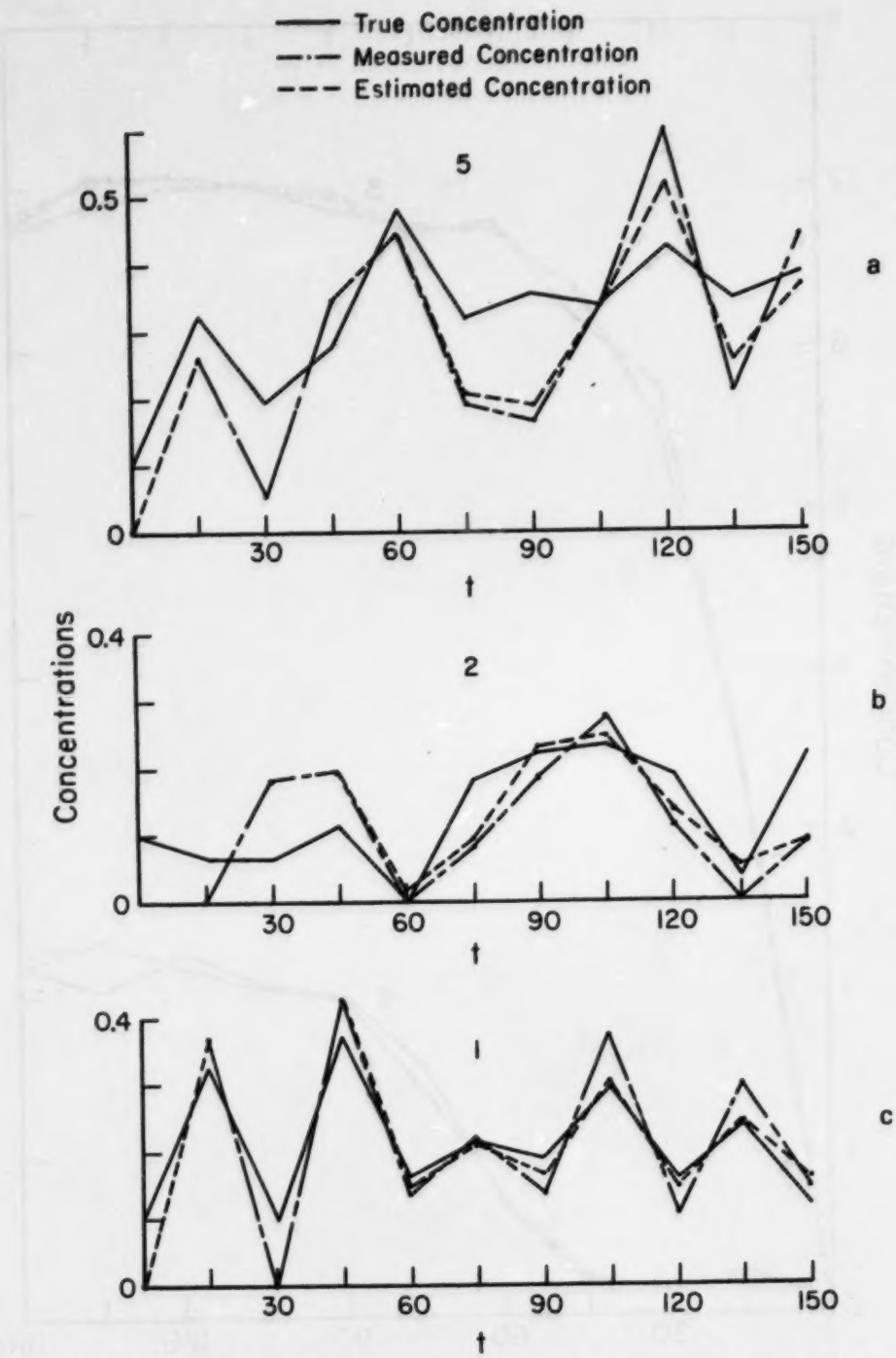


Figure 9. Comparison of estimated, true and measured concentrations, case A (a-d).

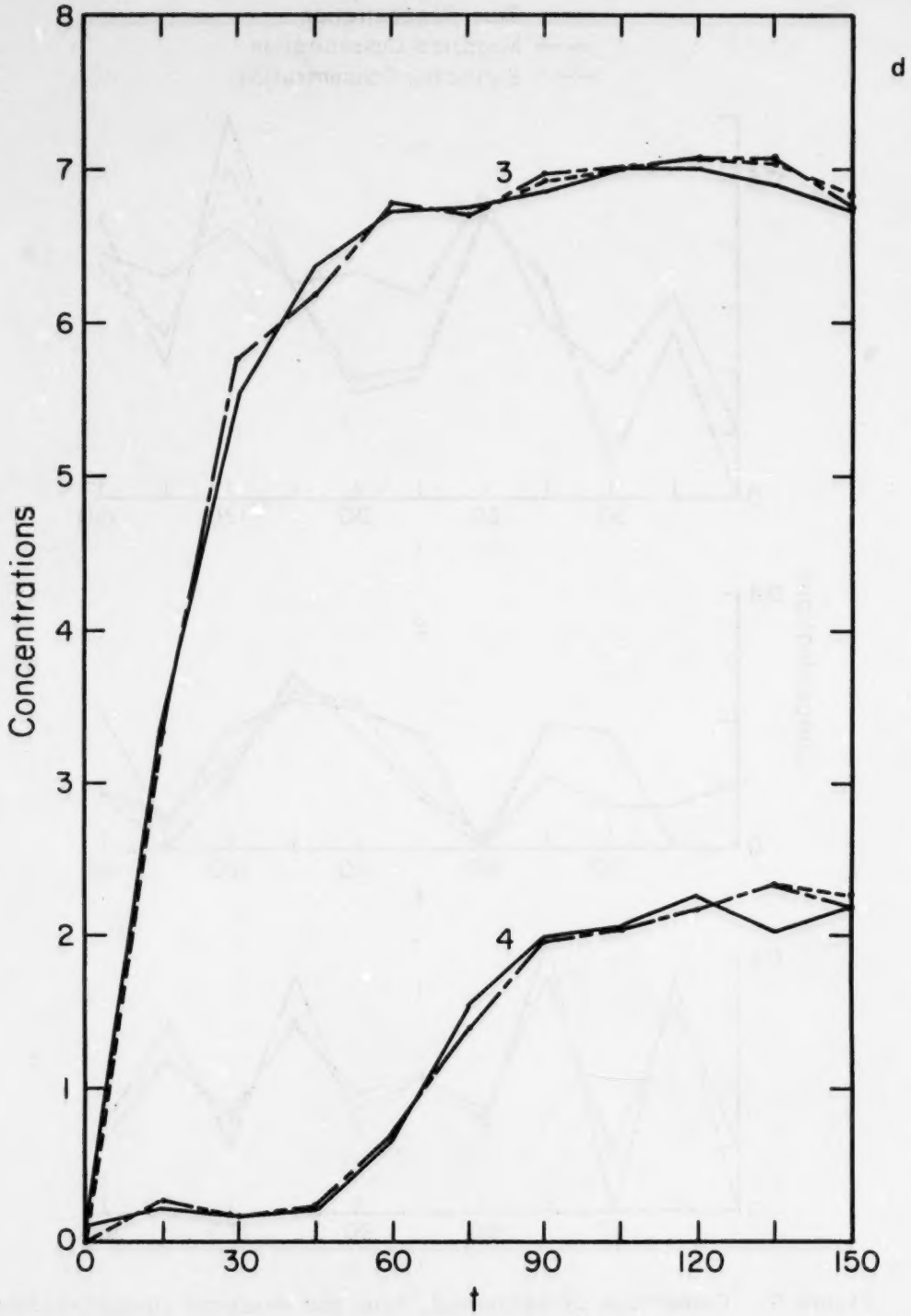


Figure 9. (continued)

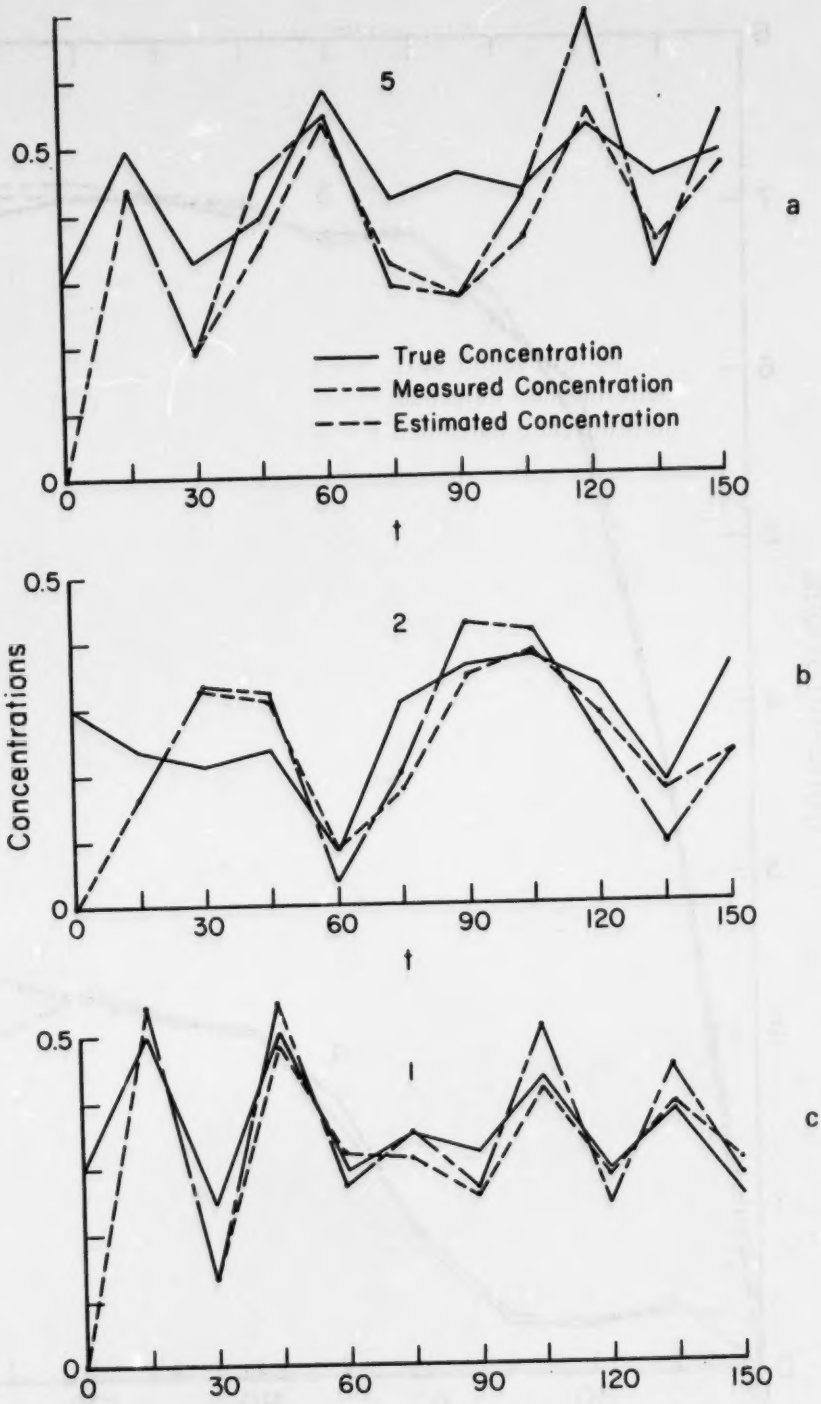


Figure 10. Comparison of estimated, true, and measured concentrations, case C (a-d).

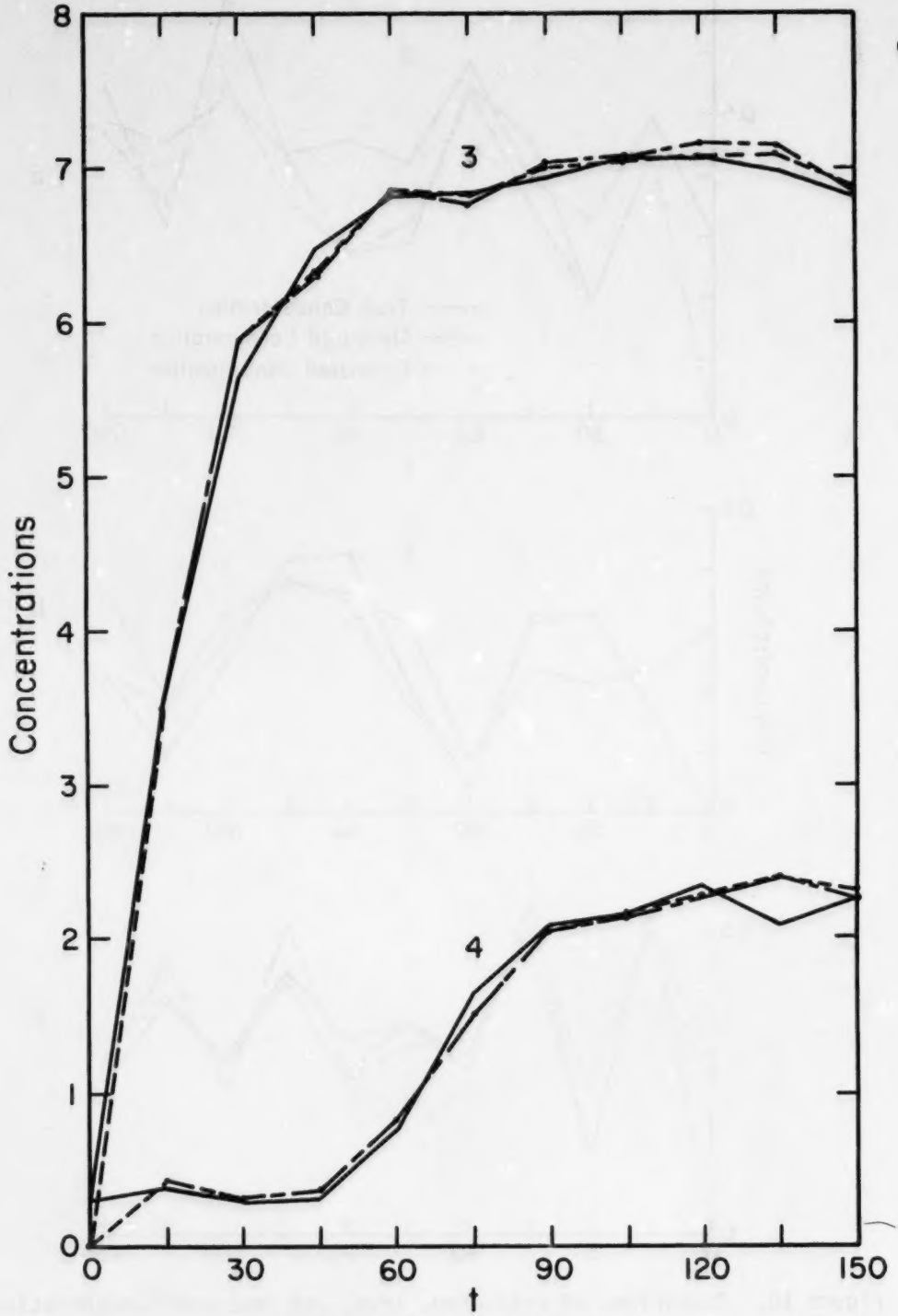
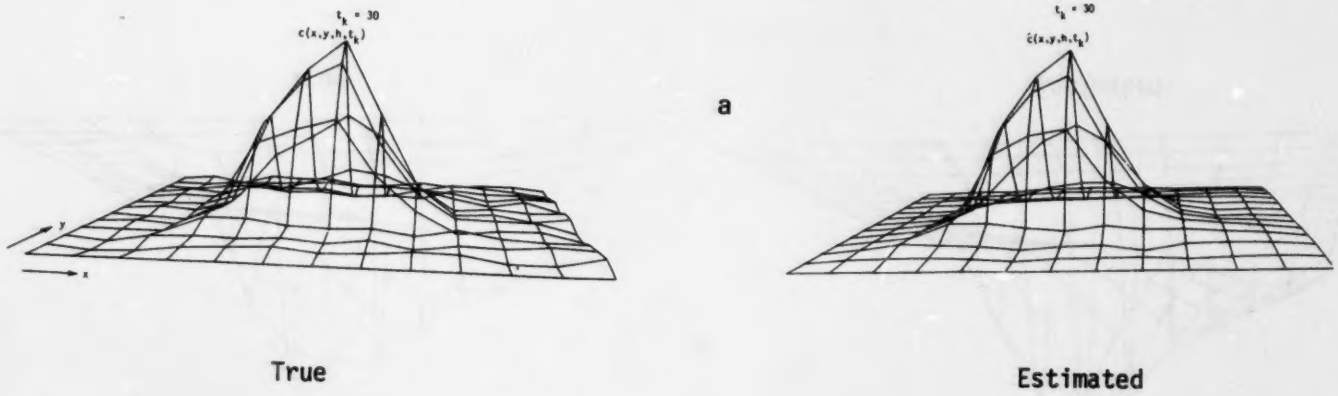


Figure 10. (continued)



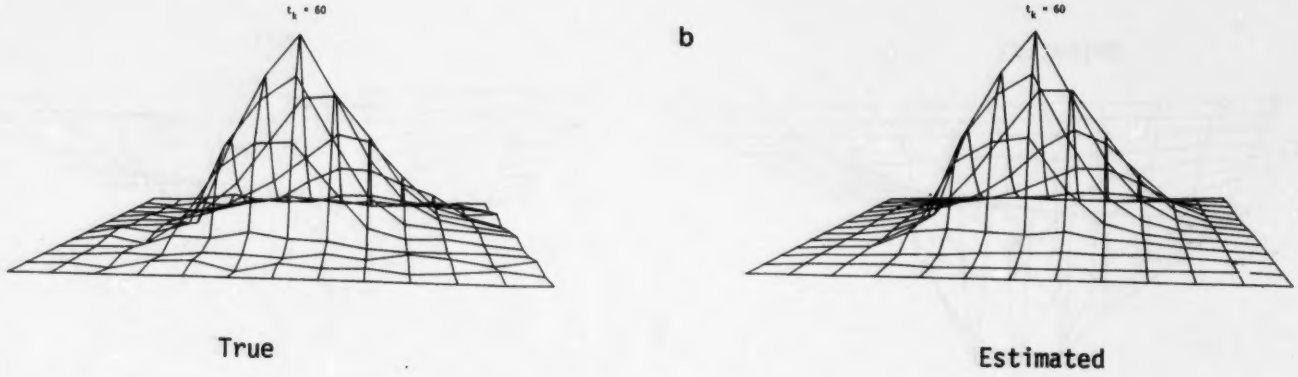
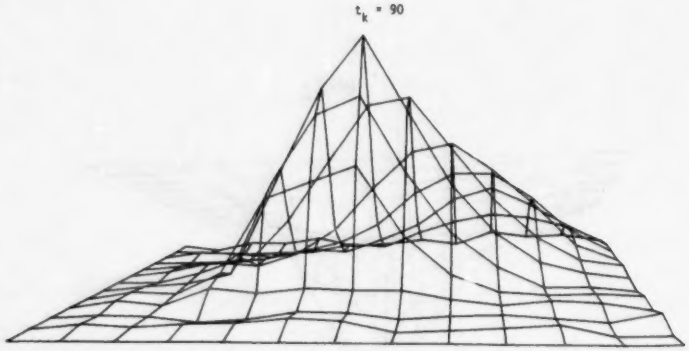
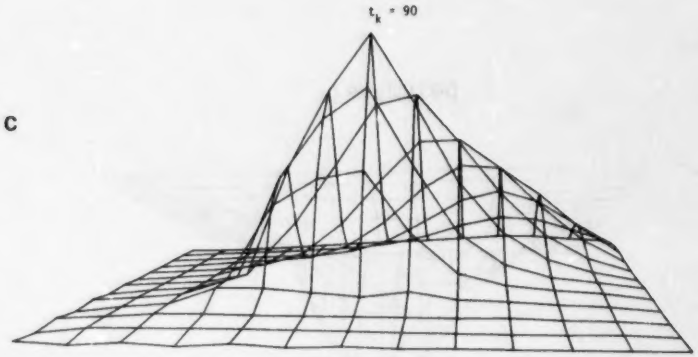


Figure 11. Comparison of spatial distributions of estimated and true concentrations, case A (a-e).

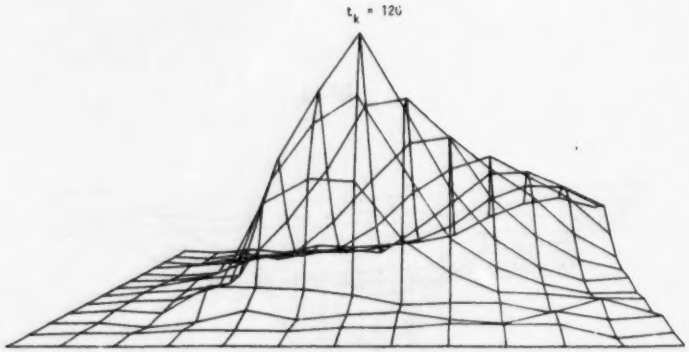


True

c

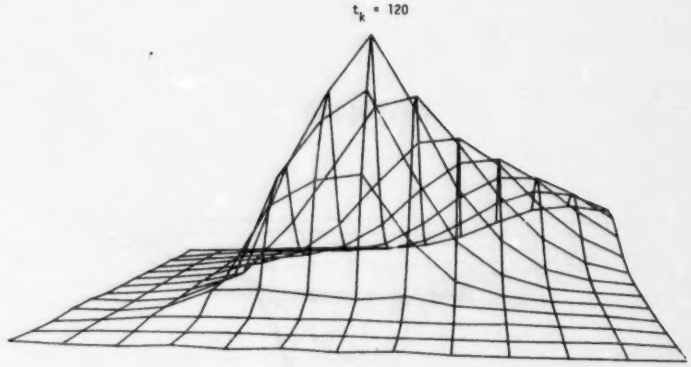


Estimated



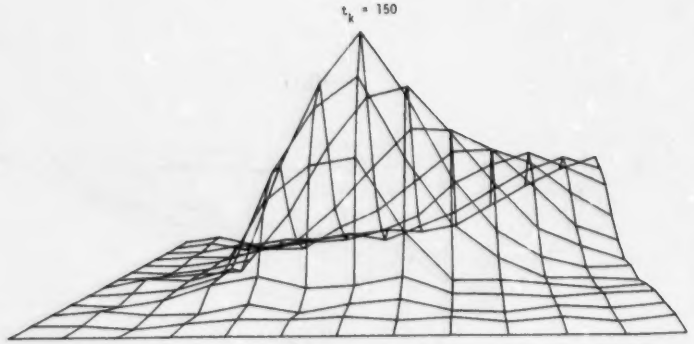
True

d



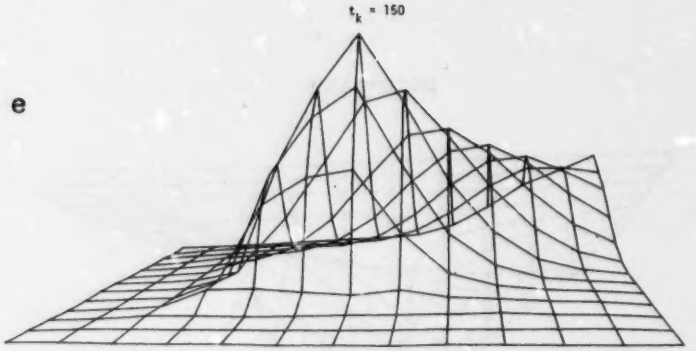
Estimated

Figure 11. (continued)



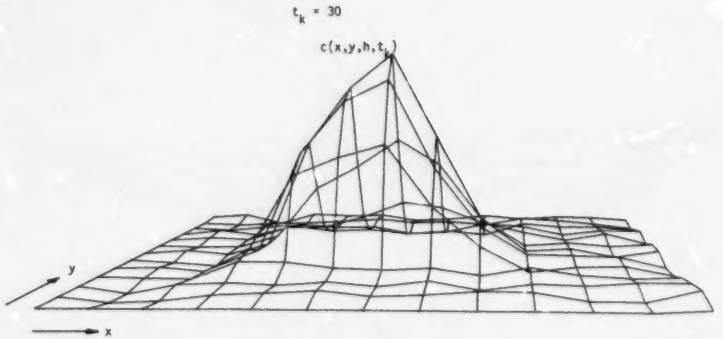
True

e



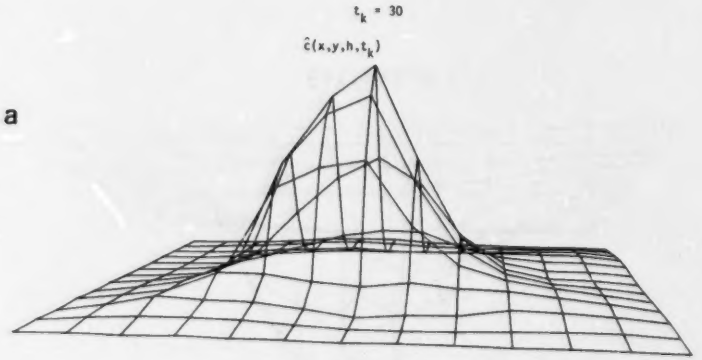
Estimated

Figure 11. (continued)



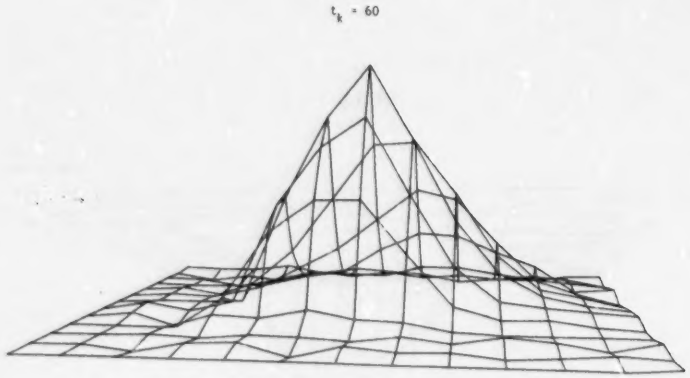
True

a



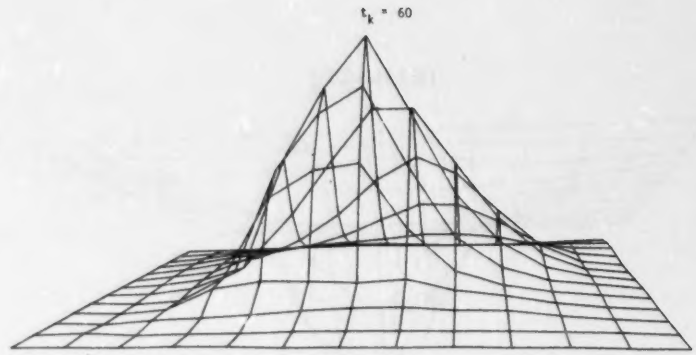
Estimated

Figure 12. Comparison of spatial distributions of estimated and true concentrations, case C (a-e).

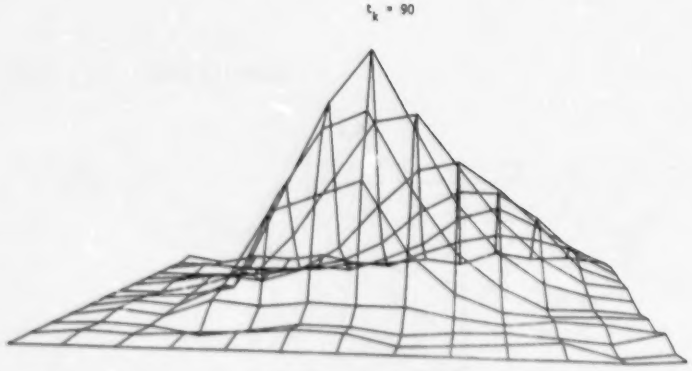


True

b

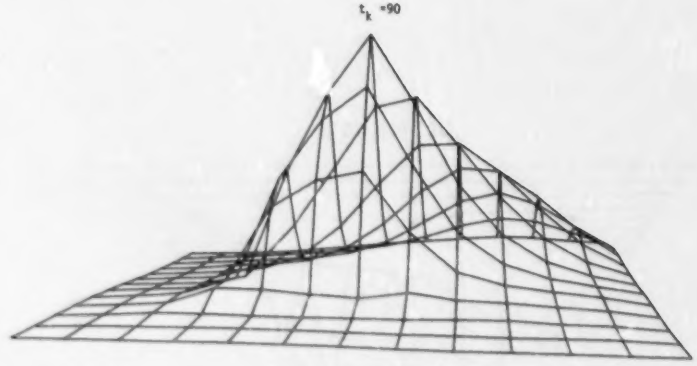


Estimated



True

c



Estimated

Figure 12. (continued)

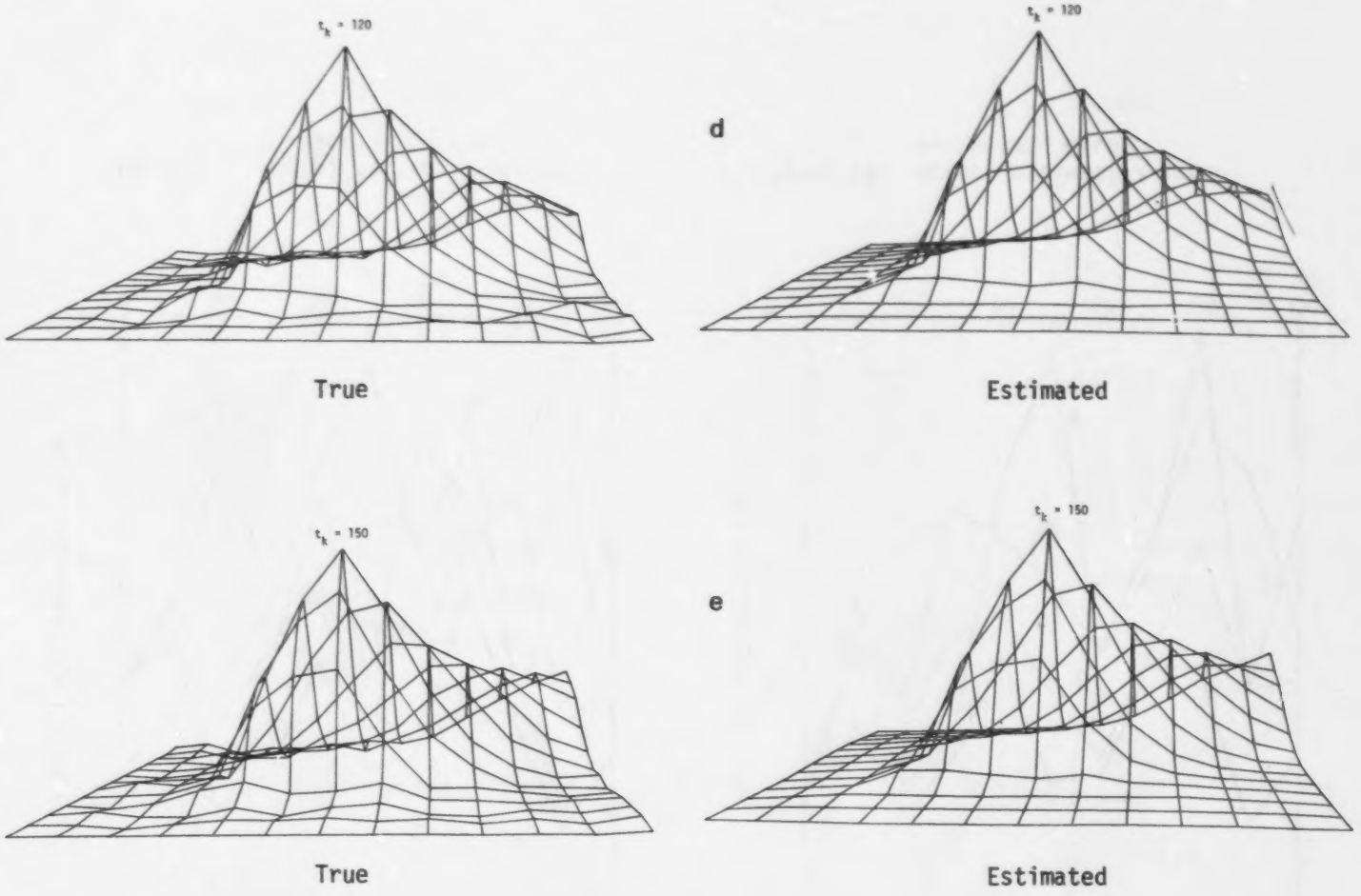


Figure 12. (continued)

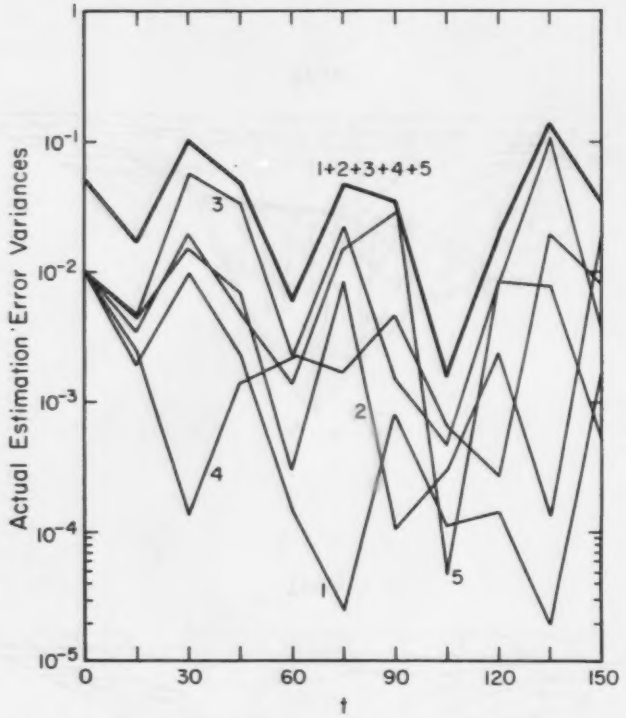


Figure 13. Actual estimation error variances, case A.

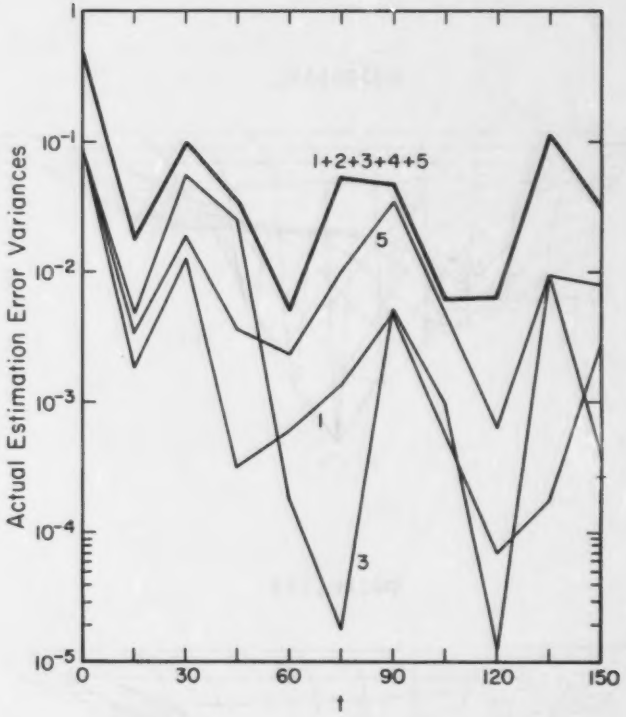


Figure 14. Actual estimation error variances, case C.

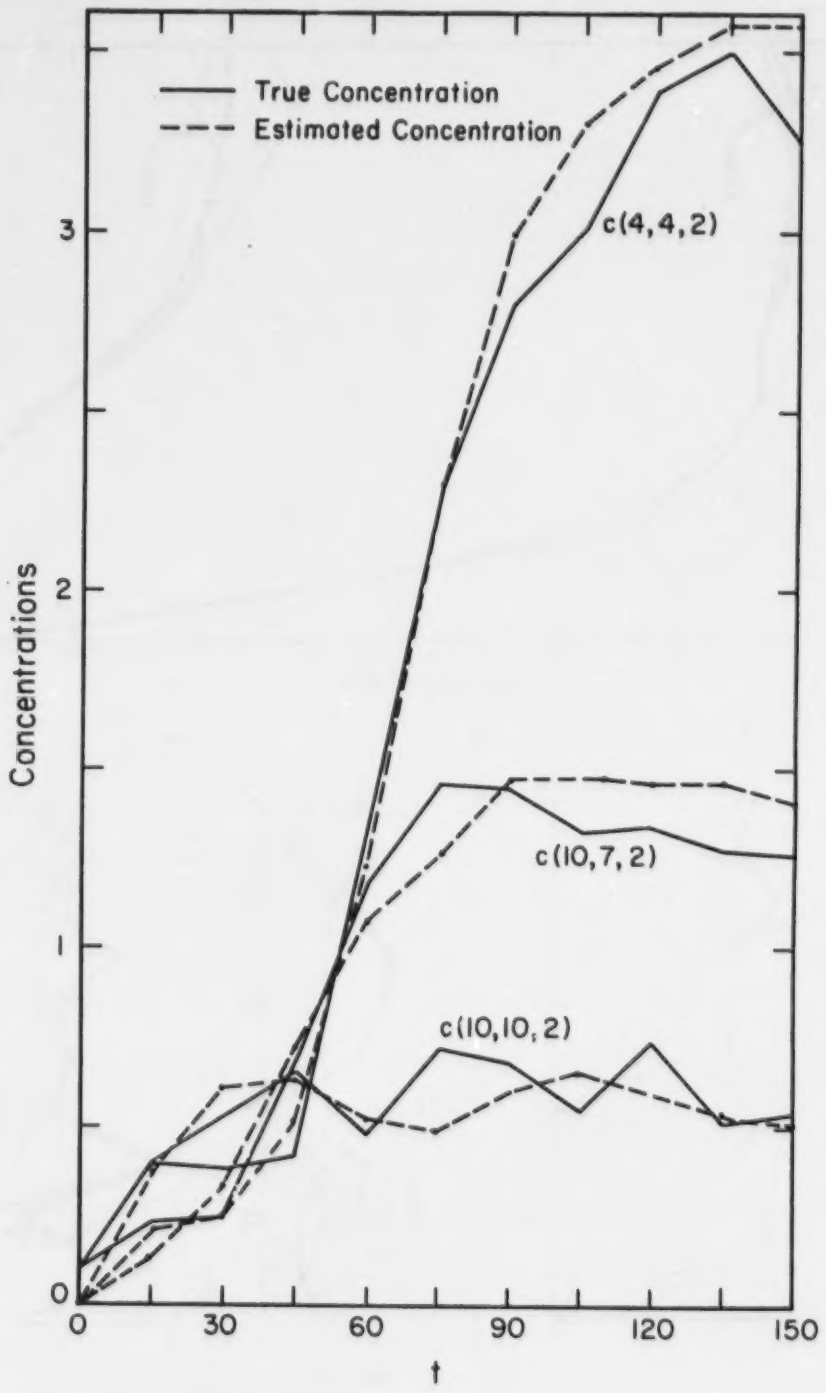


Figure 15. Comparison of estimated and true concentrations at nonmeasurement points, case A

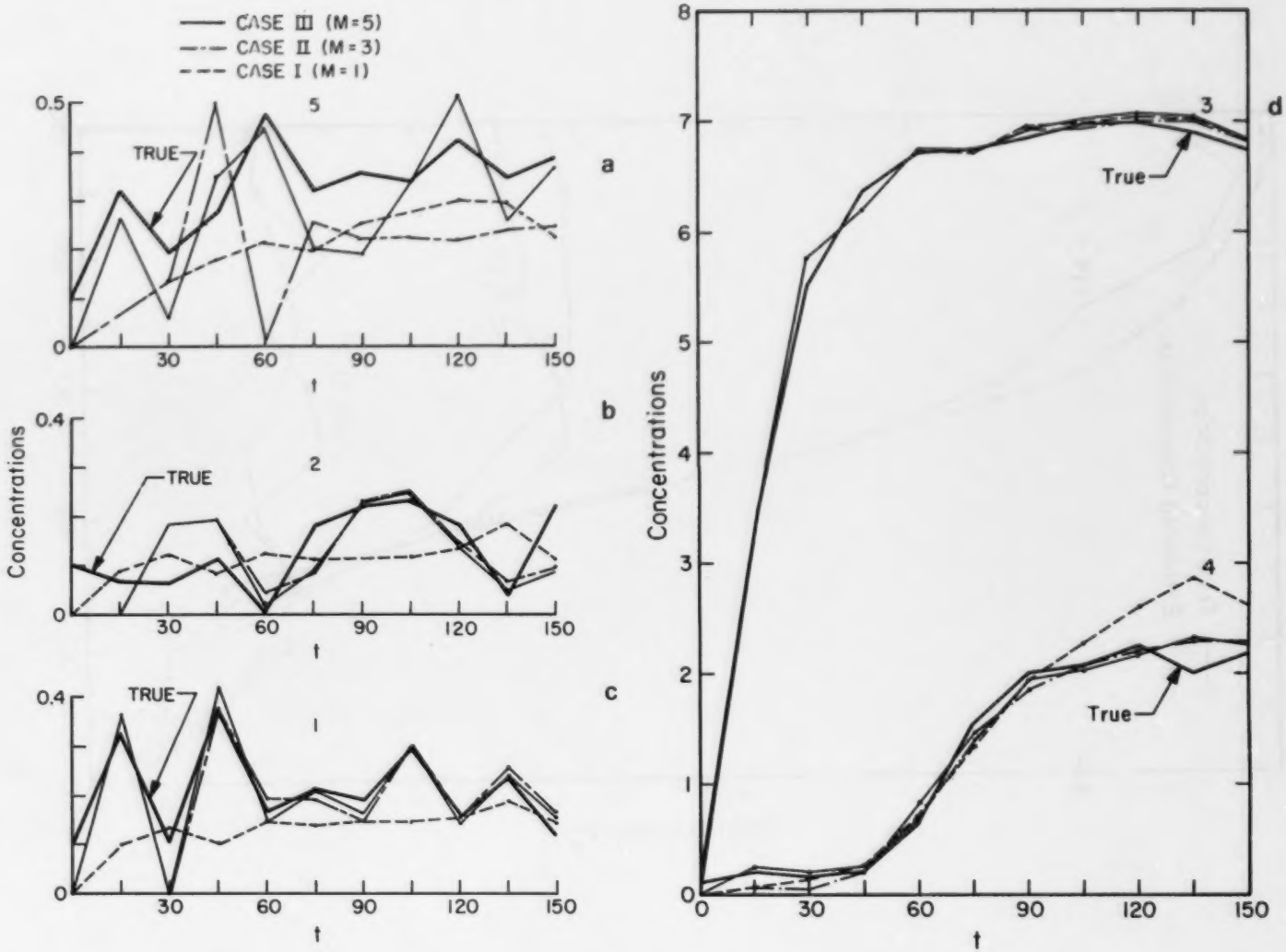


Figure 16. Comparison of estimated concentrations, base case A (a-d).

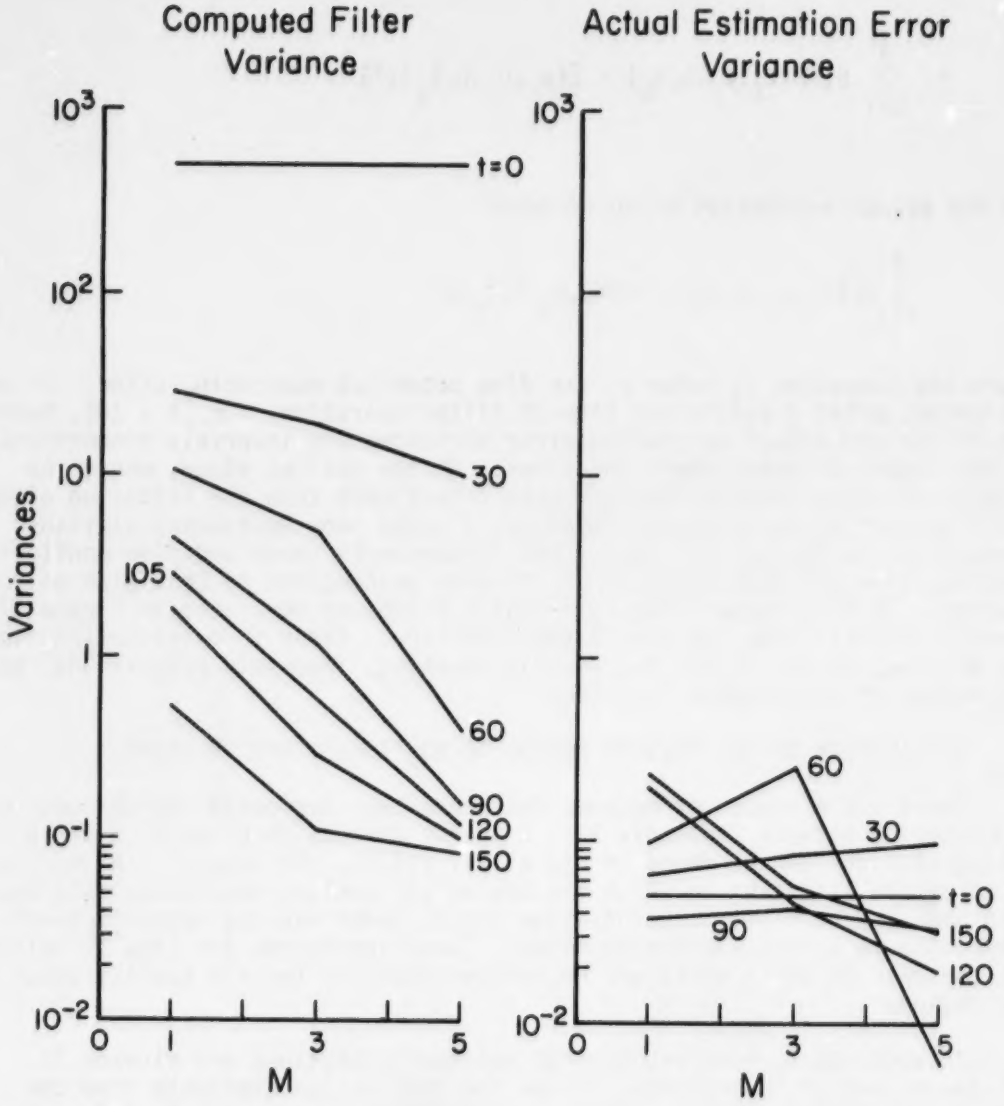


Figure 17. Comparison of variances, base case A

$$\sum_{\ell=1}^{5} P(x_\ell, y_\ell, h, x_\ell, y_\ell, h, t_k)$$

$$= \sum_{\ell=1}^{5} E\{[c(x_\ell, y_\ell, h, t_k) - \hat{c}(x_\ell, y_\ell, h, t_k)]^2\}$$

and the actual estimation error variance

$$\sum_{\ell=1}^{5} [c(x_\ell, y_\ell, h, t_k) - \hat{c}(x_\ell, y_\ell, h, t_k)]^2$$

where the summation is taken at the five potential monitoring sites. As anticipated, after a sufficient time of filter operation, i.e., $t > 105$, both the filter and actual estimation error variances are inversely proportional to the number of measurement locations. At the initial stage, where the effects of measurement errors are more significant than the filtering effects, there appears to be no great advantage in using many monitoring stations. However, after the initial stage, the filters with three and five monitoring stations show the much improved performance as compared to that with only one station. In this respect, we note that $t = 105$, as indicated in Figure 17, gives a critical time for the filter operation. After this initiation time, the accuracy of the filter is, roughly speaking, inversely proportional to the number of measurement locations.

E. APPLICATION OF THE PRESENT METHOD TO MONITOR SITING PROBLEMS

There are a number of methods that have been suggested for the design of a monitoring network (Appendix D). A useful discussion of many criteria for siting stations can be found in Liu et al. (1977). In general, the approaches focus on the situation in which one has an air quality model available and then uses the predicted concentration fields under varying meteorological conditions to select monitoring sites. These approaches are ideally suited for the case in which there are no current stations (or air quality data) in the region.

In most cases, however, several monitoring stations are already in existence, and it is desirable to use the information available from the existing stations as well as the information that can be obtained from the basic air quality model to locate new stations (or move old ones), for more effective surveillance of pollutant concentrations. The present filtering method provides the pollutant concentration distribution over an urban region by making proper use of both the limited observed data and the basic atmospheric diffusion equation. Therefore, the present method can provide the monitoring network designer with an effective computational technique to evaluate different criteria for monitor siting that require knowledge of the full concentration distribution over the region. For example, one of the

siting criteria often suggested is to locate stations at local points of maximum concentration. (For other criteria we refer the reader to Liu et al. (1977).) The evaluation of the concentration distribution can be effectively performed by making use of the present filtering algorithm. We may note, as we have already observed in Section III.B, that the filter variance is completely independent of the source emissions. This implies that the performance of the filter as a whole is quite sensitive to the large sources in the region while the filter variance, or the filter gain, is determined only by the diffusion model, i.e., wind velocity components and diffusion factors, e.g., eddy diffusivities. Thus, it is easy to take into account the occurrence of various wind field patterns and diffusion factors to reflect an impact of these factors on a potential monitor as well as a source-monitor relationship.

A problem in the application of the present method to the actual air pollution situations is the identification of the noise statistics, i.e., Q and R. As we have seen in the previous sections, the filter variance function P essentially carries all the information necessary to resolve completely the filtering problem. We have observed that P is independent of the actual data and depends only on Q and R if the initial condition is specified. Therefore, the proper identification of Q and R is very important for the present algorithm.

In general, Q determines the steady-state ($t\to\infty$) level of the filter variance. The filter variance equation with Q = 0, i.e., no dynamic noise, is notoriously unstable; it frequently gives negative diagonal entries in P. On the other hand, in situations with high dynamic noise level, the filter algorithm shows better numerical stability, but the results cannot ofen be regarded as accurate or reliable. Hence, it is clear that there are some lower and upper bounds in the choice of Q to limit the correlations within a reasonable value, e.g.,

$$0 < Q_{min} \leq Q \leq Q_{max}$$

The identification of Q is based on our judgment as to the essential adequacy of the atmospheric diffusion model for the given situation. Thus the choice of Q is problem (model) dependent and appropriate values are generally determined from prior simulation studies.

The choice of R depends on how the discrepancies between data and prediction are expected to vary with location. The identification of R can be carried out through a statistical analysis of past model validation studies. Let the predicted and observed concentrations at the monitoring time t_k and the monitoring location $\underset{\sim}{x}_i$ be given by $\hat{c}(\underset{\sim}{x}_i,t_k)$ and $c(\underset{\sim}{x}_i,t_k)$, respectively. For a series of N model runs, we can form R at each t_k as

$$R_{ij}(t_k) = \frac{1}{N}\sum_{n=1}^{N}[c(\underset{\sim}{x}_i,t_k) - \hat{c}(\underset{\sim}{x}_i,t_k)]_n[c(\underset{\sim}{x}_j,t_k) - \hat{c}(\underset{\sim}{x}_j,t_k)]_n$$

where the subscript n denotes the realization at n-th model run. Thus, these identification problems involve the off-line statistical data analysis based on the air quality model.

At present the resources required for the computer time and storage requirements for a realistic situation would be prohibitive for most air pollution control agencies. In the test situation considered here, large computer costs and storage were required when only a 13x13 mesh was used to represent the region. Increases in both would occur as the mesh points increase in number.

Techniques for estimating the mean concentration field over a region given sparse measurements have also been developed using more simplified interpolation procedures such as the inverse of some power of distance and the calculus of variations (see Appendix D). It is desirable to compare results from the relatively sophisticated scheme developed in this work and simpler, less expensive, techniques such as those discussed in Appendix D in relation to the improvement achieved per unit of resource expended.

SECTION IV

CONCLUSIONS

This study is an investigation of the application of estimation (filtering) theory to air pollution. In particular, we have explored the use of filtering algorithms to estimate the distribution of air pollutant concentrations. The estimated concentration distribution is then used for the siting of additional monitoring stations.

The specific conclusions of this study are:

1. The filter is able to produce estimates that follow the changes in pollutant concentrations as a function of time and location.

2. The numerical stability of the filter is not sensitive to the choice of a priori filter statistics and low noise levels.

3. The estimate uncertainty is, roughly speaking, inversely proportional to the number of measurement stations.

4. The time of filter operations and the number of measurement points are the most significant factors that determine the filter performance.

The filter is shown to produce very effectively the real-time estimation of the fine structure of the pollutant distribution over a region on the basis of sparse measurement data. The results reported herein, thus, can be effectively used in an air monitor siting study.

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APPENDIX

A. Distributed Parameter Filtering Theory

The urban atmosphere can be considered as a stochastic, distributed parameter system the state of which is the (ensemble mean) pollutant concentrations as a function of location and time. In this section we review the essential results from distributed-parameter filtering theory that are relevant to the air pollution estimation problem.

The system model consists of equation (5) with the measurement process given by equation (8). As we have noted, (5) is not the exact equation for the ensemble mean because of eddy diffusivities K_H and K_V representation of the turbulent diffusion process. We propose to add an artificial random forcing term to the right hand side of (5) to account for discrepancies between c_i as predicted by (5) and the true (but unknown) ensemble mean concentration.

The system is abstractly described by

$$\frac{\partial c(\underset{\sim}{x},t)}{\partial t} = L_x c(\underset{\sim}{x},t) + \xi(\underset{\sim}{x},t) \tag{A.1}$$

on a connected open domain Ω of an m-dimensional Euclidean space E^m, with boundary $\partial\Omega$. The m-dimensional spatial coordinate vector is denoted by $\underset{\sim}{x}$. The state $c(\underset{\sim}{x},t)$ is a scalar ensemble mean concentration, and L_x is a spatial elliptic differential operator associated with (5). The process noise $\xi(\underset{\sim}{x},t)$ is a scalar distributed white Gaussian process with properties:

$$\begin{aligned} &E\{\xi(\underset{\sim}{x},t)\} = 0 \\ &E\{\xi(\underset{\sim}{x},t)\xi(\underset{\sim}{y},\tau)\} = Q(\underset{\sim}{x},\underset{\sim}{y},t)\delta(t-\tau) \end{aligned} \tag{A.2}$$

where $Q(x,y,t)$ is symmetric with respect to the spatial variables x and y, and positive semi-definite variance function. The initial state $c(\underset{\sim}{x},t_o)$ is a white Gaussian process and only its mean $\hat{c}_o(\underset{\sim}{x})$ and variance $P_o(\underset{\sim}{x},\underset{\sim}{y})$, i.e.,

$$\begin{aligned} &E\{c(\underset{\sim}{x},t_o)\} = \hat{c}_o(\underset{\sim}{x}) \\ &E\{[c(\underset{\sim}{x},t_o) - \hat{c}_o(\underset{\sim}{x})][c(\underset{\sim}{y},t_o) - \hat{c}_o(\underset{\sim}{y})]\} = P_o(\underset{\sim}{x},\underset{\sim}{y}) \end{aligned} \tag{A.3}$$

are assumed to be known. The boundary conditions have been assumed to be inhomogeneous,

$$L_b c(\underset{\sim}{x},t) = \phi(\underset{\sim}{x},t) \qquad , \underset{\sim}{x} \in \partial\Omega \tag{A.4}$$

where L_b is a linear boundary differential operator and $\phi(\underset{\sim}{x},t)$ is a known deterministic function. It is clear that (5) falls within the class (A.1), and there is no loss of generality in assuming, in this discussion, that the state and other functions are scalar.

The measurement process is represented as

$$w_\ell(t_k) = c(\underset{\sim}{x}_\ell,t_k) + \eta_\ell(t_k) \qquad , \quad \ell = 1,2,\ldots, M \tag{A.5}$$

where $\eta_\ell(t_k)$ is a white Gaussian process with properties:

$$E\{\eta_i(t_n)\} = 0$$

$$E\{\eta_i(t_m)\eta_j(t_n)\} = R_{ij}(t_n)\delta_{mn} \tag{A.6}$$

where $R_{ij}(t_n)$ is a positive variance. It is important to note that (A.5) represents the most important class of measurement situations in the air pollution estimation problem, i.e., discrete-time measurements at M-discrete points in space.

The filtering problem is as follows:

> Given a realization $\{w_\ell(t_k),\ \ell = 1,2,\ldots, M;\ k = 1,2,\ldots\}$, find the estimate of the state $c(\underset{\sim}{x},t)$ that maximizes the conditional probability density functional of the state.

This optimal estimation problem can be solved most effectively by using the maximum likelihood approach based on the theory of the semigroup of linear operators in Hilbert space. We now discuss briefly the optimal solution of the linear distributed filtering problem.

First we consider the time update equations, i.e., equations which describe the time evolution of the filter state between measurements. Since there is no additional information between the measurements, the maximization of the conditional probability is achieved by simply taking the expectation of the state. Hence, from (A.1) and (A.4), the following time update equations hold for the optimal estimate $\hat{c}(\underset{\sim}{x},t)$,

$$\frac{\partial \hat{c}(\underset{\sim}{x},t)}{\partial t} = L_x \hat{c}(\underset{\sim}{x},t) \qquad t_k < t \leq t_{k+1} \tag{A.7}$$

$$L_b \hat{c}(\underset{\sim}{x},t) = \phi(\underset{\sim}{x},t) \qquad , \ \underset{\sim}{x} \in \partial\Omega \tag{A.8}$$

The estimation error

$$\tilde{c}(\underset{\sim}{x},t) = c(\underset{\sim}{x},t) - \hat{c}(\underset{\sim}{x},t) \tag{A.9}$$

has the variance defined by

$$P(\underset{\sim}{x},\underset{\sim}{y},t) = E\{\tilde{c}(\underset{\sim}{x},t)\tilde{c}(\underset{\sim}{y},t)\} \tag{A.10}$$

By definition, the variance function $P(\underset{\sim}{x},\underset{\sim}{y},t)$ is symmetric with respect to $\underset{\sim}{x}$ and $\underset{\sim}{y}$ and positive semi-definite.

Subtracting (A.7) and (A.8) from (A.1) and (A.4) respectively, we can obtain the following equations for the estimation error $c(\underset{\sim}{x},t)$.

$$\frac{\partial \tilde{c}(\underset{\sim}{x},t)}{\partial t} = L_x \tilde{c}(\underset{\sim}{x},t) + \xi(\underset{\sim}{x},t) \qquad t_k < t \leq t_{k+1} \tag{A.11}$$

$$L_b \tilde{c}(\underset{\sim}{x},t) = 0 \quad , \qquad \underset{\sim}{x} \in \partial\Omega \tag{A.12}$$

It is important to note that the estimation error satisfies the homogeneous boundary condition (A.12) while the optimal estimate satisfies the inhomogeneous boundary condition (A.8). The general solution of (A.11) with homogeneous boundary condition (A.12) can be expressed in the form:

$$\tilde{c}(\underset{\sim}{x},t) = \int_{\Omega} G(\underset{\sim}{x},t;\underset{\sim}{y},t')\tilde{c}(\underset{\sim}{y},t')\, d\underset{\sim}{y}$$

$$+ \int_{t'}^{t}\int_{\Omega} G(\underset{\sim}{x},t;\underset{\sim}{y},\tau)\xi(\underset{\sim}{y},\tau)\, d\underset{\sim}{y}d\tau \tag{A.13}$$

where t' is a suitable initial time and $G(\underset{\sim}{x},t;\underset{\sim}{y},\tau)$ is the Green's function associated with (A.11) and (A.12). Note that $G(\underset{\sim}{x},t;\underset{\sim}{y},\tau)$ satisfies the equation,

$$\frac{\partial}{\partial t} G(\underset{\sim}{x},t;\underset{\sim}{y},\tau) = L_x G(\underset{\sim}{x},t;\underset{\sim}{y},\tau) \tag{A.14}$$

with the terminal condition

$$G(\underset{\sim}{x},t';\underset{\sim}{y},t') = \delta(\underset{\sim}{x} - \underset{\sim}{y}) \tag{A.15}$$

and boundary condition

$$L_b G(\underset{\sim}{x},t;\underset{\sim}{y},\tau) = 0 \ , \qquad \underset{\sim}{x} \in \partial\Omega \tag{A.16}$$

Using (A.13) with (A.10) we obtain the estimation error variance function as

$$P(\underset{\sim}{x},\underset{\sim}{y},t) = \iint_{\Omega\Omega} G(\underset{\sim}{x},t;\underset{\sim}{r},t')P(\underset{\sim}{r},\underset{\sim}{s},t')G(\underset{\sim}{y},t;\underset{\sim}{s},t')\, d\underset{\sim}{r}d\underset{\sim}{s}$$

$$+ \int_{t'}^{t} \iint_{\Omega\Omega} G(\underset{\sim}{x},t;\underset{\sim}{r},\tau)Q(\underset{\sim}{r},\underset{\sim}{s},\tau)G(\underset{\sim}{y},t;\underset{\sim}{s},\tau)\, d\underset{\sim}{r}d\underset{\sim}{s}d\tau \qquad \text{(A.17)}$$

Formal differentiation of (A.17) with respect to t together with the use of (A.14) - (A.16) gives the following differential equations for the estimation error variance:

$$\frac{\partial P(\underset{\sim}{x},\underset{\sim}{y},t)}{\partial t} = L_x P(\underset{\sim}{x},\underset{\sim}{y},t) + P(\underset{\sim}{x},\underset{\sim}{y},t)L_y' + Q(\underset{\sim}{x},\underset{\sim}{y},t) \qquad \text{(A.18)}$$

$$L_b P(\underset{\sim}{x},\underset{\sim}{y},t) = 0 \quad , \quad \underset{\sim}{x} \in \partial\Omega \qquad \text{(A.19)}$$

$$P(\underset{\sim}{x},\underset{\sim}{y},t)\, L_b' = 0 \quad , \quad \underset{\sim}{y} \in \partial\Omega \qquad \text{(A.20)}$$

where the formal operator L_y' is defined by the relation $P(\underset{\sim}{x},\underset{\sim}{y},t)L_y' = L_y P(\underset{\sim}{x},\underset{\sim}{y},t)$, and is an operator to the left. The same definition is utilized for L_b'. Thus it has been shown that the variance function $P(\underset{\sim}{x},\underset{\sim}{y},t)$ has the homogeneous boundary conditions (A.19) and (A.20).

It is important to note that the predicted (a priori) information at the start of the measurement interval coincides with the filtered results before any data have been included. This explains the initialization of the time update equations: initial conditions of (A.7) and (A.18) should be filtered (a posteriori) estimate and variance, respectively.

At each measurement instant, the solution to (A.7) with boundary condition (A.8), and the solution to (A.18) with boundary conditions (A.19) and (A.20) constitute the current estimate and variance. These become a priori (predicted) estimates and are combined with the new data at $t=t_{k+1}$ to update the estimate and variance. The equation defining the optimal estimate at measurement instant time t_{k+1} is

$$\hat{c}(\underset{\sim}{x},t_{k+1}^{+}) = \hat{c}(\underset{\sim}{x},t_{k+1}^{-}) + \sum_{i=1}^{M}\sum_{j=1}^{M} P(\underset{\sim}{x},\underset{\sim}{s}_i,t_{k+1}^{-})[\Lambda^{-1}(t_{k+1})]_{ij}$$

$$\cdot[w_j(t_{k+1}) - \hat{c}(\underset{\sim}{s}_j,t_{k+1}^{-})] \qquad \text{(A.21)}$$

where the superscripts - and + denote the time instants immediately prior to and immediately subsequent to the measuring instant, respectively. Note that $c(\underset{\sim}{x},t_{k+1}^{-})$ is a solution to (A.7) and (A.8) at t_{k+1}. The variance function $P(\underset{\sim}{x},\underset{\sim}{y},t)$ obeys the following equation at the measurement instant t_{k+1}:

$$P(\underset{\sim}{x},\underset{\sim}{y},t_{k+1}^{+}) = P(\underset{\sim}{x},\underset{\sim}{y},t_{k+1}^{-})$$

$$- \sum_{i=1}^{M}\sum_{j=1}^{M} P(\underset{\sim}{x},\underset{\sim}{s}_i,t_{k+1}^{-})[\Lambda^{-1}(t_{k+1})]_{ij}P(\underset{\sim}{s}_j,\underset{\sim}{y},t_{k+1}^{-}) \qquad (A.22)$$

Note that $P(\underset{\sim}{x},\underset{\sim}{y},t_{k+1}^{-})$ is a solution to (A.18), (A.19), and (A.20). The matrix $\underset{\sim}{\Lambda}(t_{k+1})$ in (A.21) and (A.22) is defined by its element as

$$[\Lambda(t_{k+1})]_{ij} = P(\underset{\sim}{s}_i,\underset{\sim}{s}_j,t_{k+1}^{-}) + R_{ij}(t_{k+1}) \qquad (A.23)$$

It is important to note that (A.22) does not depend on the actual measurements. Hence, we can quite routinely generate variance functions corresponding to candidate air pollution models and measurement strategies. In this way estimation accuracy might be determined prior to the occurrence of the actual event.

B. Finite Difference Approximation and Square Root Implementation of Distributed Parameter Filter

The major impediment to the application of distributed parameter filtering is the spatial dimensionality of the filter. If m=3 (most general air pollution problems have three spatial variables), then the filter variance $P(x,y,t)$ is a function of six spatial variables. Numerical solutions of partial differential and/or difference equations having more than three spatial dimensions are rarely attempted, particularly for equations as complex as the variance Riccati equation of the distributed parameter filter. The key problem, therefore, in the application of distributed parameter filtering to air pollution analysis, is the development of efficient methods for solving the variance equations of the filter.

B.1 Finite Difference Approximation of Distributed Parameter Filter

Approximation of the filter is, of course, required at some point since distributed parameter systems span an infinite-dimensional space and it is only possible numerically to obtain solutions in a finite-dimensional subspace. In order to work with the solutions of the filter, we develop a finite difference approximation.

In discussing the finite difference approximation it is useful to consider a specific form of the atmospheric diffusion equation. If turbulent diffusion in the horizontal directions and vertical wind velocity component can be neglected, the atmospheric diffusion equation, with the addition of a dynamic error, becomes

$$\frac{\partial c}{\partial t} + u(z)\frac{\partial c}{\partial x} + v(z)\frac{\partial c}{\partial y} = \frac{\partial}{\partial z}\left\{K_V(z)\frac{\partial c}{\partial z}\right\} + \xi(x,y,z,t) \qquad (B.1)$$

where $x \in [0, X_{max}]$, $y \in [0, Y_{max}]$, and $z \in [0, Z_{max}]$. The boundary conditions are given by,

$$-K_{vo}\frac{\partial c(x,y,0,t)}{\partial z} = S(x,y,t)$$

$$\frac{\partial c(x,y,Z_{max},t)}{\partial z} = 0 \qquad (B.2)$$

where $S(x,y,t)$ is the surface flux of the pollutant. Other boundary conditions are given at the upwind boundaries:

$$c(0,y,z,t) = c_b$$

$$c(x,0,z,t) = c_b \qquad (B.3)$$

where c_b can be a function of time.

Let $\Delta x = X_{max}/N_x$, $\Delta y = Y_{max}/N_y$, and $\Delta z = Z_{max}/N_z$, where N_x, N_y, and N_z are the numbers of mesh points in the x,y,z directions, respectively, and let Δt be a suitable finite difference time step. Let us denote $x_i = i\Delta x$, $y_j = j\Delta y$, $z_k = k\Delta z$, and $t_\sigma = \sigma\Delta t$. We shall use the following notation:

$$g^{\sigma}_{ijk} = g(x_i, y_j, z_k, t_\sigma)$$

$$g^{\sigma,\theta}_{ijk} = \frac{1}{2}(1-\theta)g^{\sigma+1}_{ijk} + \frac{1}{2}(1+\theta)g^{\sigma}_{ijk} \qquad (B.4)$$

where $\theta \in [0,1]$ and let δ_t denote the forward difference operator:

$$\delta_t g^{\sigma}_{ijk} = (g^{\sigma+1}_{ijk} - g^{\sigma}_{ijk})/\Delta t \ . \qquad (B.5)$$

Based on the present model (B.1), we can construct a family of finite difference approximations associated with parameter θ which represent solutions to the state time update equation (A.7):

$$\delta_t \hat{c}^{\sigma}_{ijk} = - L_1(k) \sum_{\nu=1}^{N_x} A^{(1)}_{i\nu} \hat{c}^{\sigma,\theta}_{\nu jk} - L_2(k) \sum_{\nu=1}^{N_y} A^{(2)}_{j\nu} \hat{c}^{\sigma,\theta}_{i\nu k}$$

$$+ L_3(k) \sum_{\nu=1}^{N_z} A^{(3)}_{k\nu} \hat{c}^{\sigma,\theta}_{ij\nu} \qquad \text{(B.6)}$$

$$i = 1,\ldots, N_x \; ; \; j = 1,\ldots, N_y \; ; \; k = 1,\ldots, N_z$$

where

$$L_1(k) = u(z_k)$$

$$L_2(k) = v(z_k) \qquad \text{(B.7)}$$

$$L_3(k) = K_V(z_k) + \frac{\partial K_V(z_k)}{\partial z}$$

The superscripts (1), (2), and (3) on the coefficient matrix $\underset{\sim}{A}$ refer to the x, y, and z coordinate directions, respectively. If $\theta = 0$, (B.6) yields the so-called Crank-Nicolson method; for $\theta = 1$, (B.6) is a simple forward difference method. The fully discrete equation (B.6) requires the solution of a system of $N_x \times N_y \times N_z$ linear algebraic equations at each time level.

In order to ascertain the stability and accuracy of the approximation, we apply the time-splitting technqiue in the actual implementation of (B.6). The technique consists of applying each 1-dimensional finite difference method independently and in succession, with no significance attached to the result of the former calculation step. In this framework the original finite difference approximation (B.6) might be decomposed into the 2-dimensional "advection part," and into the 1-dimensional "diffusion part."

(a) Advection part:

$$\delta_t^{1/3} \hat{c}^{\sigma}_{ijk} = - L_1(k) \sum_{\nu=1}^{N_x} A^{(1)}_{i\nu} \hat{c}^{\sigma,\theta}_{\nu jk} \qquad \text{(B.8)}$$

$$\delta_t^{1/3} \hat{c}^{\sigma+1/3}_{ijk} = - L_2(k) \sum_{\nu=1}^{N_y} A^{(2)}_{j\nu} \hat{c}^{\sigma+1/3,\theta}_{i\nu k} \qquad \text{(B.9)}$$

(b) Diffusion part:

$$\delta_t^{1/3} \hat{c}^{\sigma+2/3}_{ijk} = L_3(k) \sum_{\nu=1}^{N_z} A^{(3)}_{k\nu} \hat{c}^{\sigma+2/3,\theta}_{ij\nu} \qquad \text{(B.10)}$$

where $\delta_t^{1/3}$ is a difference operator defined by

$$\delta_t^{1/3} g_{ijk}^{\sigma} = (g_{ijk}^{\sigma+1/3} - g_{ijk}^{\sigma})/\Delta t \qquad (B.11)$$

This decomposition is consistent and also improves the numerical stability and accuracy. In other words, the time-splitting approach decomposes the original 3-dimensional finite difference equation into a simpler and better conditioned 1-dimensional finite difference equation.

The standard Crank-Nicolson second-order method is applied to the diffusion part (B.10). This implies $\theta = 0$ in (B.10), and the method is unconditionally stable. Fromm's (1968) second-order, zero-average phase error method is applied to the advection part (B.8) and (B.9). Then (B.8) and (B.9) can be represented as:

$$\hat{c}_{ijk}^{\sigma+1/3} = \hat{c}_{ijk}^{\sigma} + \frac{1}{4}\,\alpha_k(\hat{c}_{i-1,j,k}^{\sigma} - \hat{c}_{i+1,j,k}^{\sigma} + \hat{c}_{i-2,j,k}^{\sigma} - \hat{c}_{ijk}^{\sigma})$$

$$+ \frac{1}{4}\,(\alpha_k)^2(\hat{c}_{i-1,j,k}^{\sigma} - 2\hat{c}_{ijk}^{\sigma} + \hat{c}_{i+1,j,k}^{\sigma})$$

$$+ \frac{1}{4}\left\{(\alpha_k)^2 - 2\alpha_k\right\}(\hat{c}_{i-2,j,k}^{\sigma} - 2\hat{c}_{i-1,j,k}^{\sigma} + \hat{c}_{ijk}^{\sigma}) \qquad (B.12)$$

$$\hat{c}_{ijk}^{\sigma+2/3} = \hat{c}_{ijk}^{\sigma+1/3} + \frac{1}{4}\,\beta_k(\hat{c}_{i,j-1,k}^{\sigma+1/3} - \hat{c}_{i,j+1,k}^{\sigma+1/3} + \hat{c}_{i,j-2,k}^{\sigma+1/3} - \hat{c}_{ijk}^{\sigma+1/3})$$

$$+ \frac{1}{4}\,(\beta_k)^2(\hat{c}_{i,j-1,k}^{\sigma+1/3} - 2\hat{c}_{ijk}^{\sigma+1/3} + \hat{c}_{i,j+1,k}^{\sigma+1/3})$$

$$+ \frac{1}{4}\left\{(\beta_k)^2 - 2\beta_k\right\}(\hat{c}_{i,j-2,k}^{\sigma+1/3} - 2\hat{c}_{i,j-1,k}^{\sigma+1/3} + \hat{c}_{ijk}^{\sigma+1/3}) \qquad (B.13)$$

where $\alpha_k = u(z_k)\Delta t/\Delta x$ and $\beta_k = v(z_k)\Delta t/\Delta y$. The method is stable for $\alpha_k + \beta_k \leq 1$, and improves the phase error properties considerably. We note that the boundary conditions (B.2) and (B.3) can be easily incorporated into these finite difference equations.

The numerical procedure (B.8) - (B.10) can be formally combined so that the time update equation for the optimal estimate can be written as follows:

$$\hat{\underset{\sim}{c}}(\sigma + 1) = \underset{\sim}{\Phi}(\sigma + 1,\sigma)\hat{\underset{\sim}{c}}(\sigma) \qquad (B.14)$$

where $\hat{\underset{\sim}{c}}(\sigma)$ is the $N_x \times N_y \times N_z$-dimensional state vector with elements $\hat{c}_{ijk}^{\sigma}$, and $\underset{\sim}{\Phi}(\sigma + 1,\sigma)$ is the corresponding state transition matrix associated with the finite difference routine (B.8) - (B.10). It is important to note that (B.14) is a completely formal expression, and that, in the actual calculation, neither computation nor storage of $\underset{\sim}{\Phi}(\sigma + 1,\sigma)$ is required.

Using similar notation as in (B.14), the measurement process (A.5) can be represented in vector form as:

$$\underset{\sim}{w}(\sigma) = \underset{\sim}{H}(\sigma)\underset{\sim}{c}(\sigma) + \underset{\sim}{\eta}(\sigma) \tag{B.15}$$

where $\underset{\sim}{w}(\sigma)$ is the M-dimensional measurement vector, $H(\sigma)$ is the suitably defined $M \times N_x N_y N_z$ measurement matrix, and $\underset{\sim}{\eta}(\sigma)$ is the M-dimensional white Gaussian sequence with the covariance matrix $\underset{\sim}{R}(\sigma)$ whose elements are defined by $R_{ij}(t_\sigma)$ in (A.6).

B.2 Square Root Implementation of Distributed Parameter Filter

The finite difference method may be also effectively applied to the time update equation for the estimation error variance. The basic problem in this approach lies in the dimensionality of the filter variance equation (A.18), for which extensive numerical computations are necessary.

Usually large-dimensioned systems are overly sensitive to numerical errors and the effects of numerical errors are generally manifested in various type of numerical difficulties. Difficulties relating to computer roundoff appeared in even the very early applications of Kalman filtering procedure. Numerics is the dominant error source in the Kalman algorithms, and they completely obscured the important effects of mismodeling and lead to misleading estimates of the filter accuracy.

The measurement update equation of the filter variance (A.22) is sensitive to the effects of computer roundoff and is susceptible to an accuracy degradation due to the differencing of positive terms. This numerical accuracy degradation is often accompanied by a computed variance that loses its positive definiteness. An alternative and more consistently reliable solution to the numerical instability problem is to perform some of the computations using an algorithm that is numerically better conditioned. As such an alternative we utilize the square root implementation of the filter variance equations.

The direct application of the finite difference routine to the variance equation (A.18) results in the following expression (using the same notation of Section B.1.):

$$\begin{aligned}
\delta_t P^{\sigma}_{ijk\ell mn} = &- L_1(k) \sum_{\nu=1}^{N_x} A^{(1)}_{i\nu} P^{\sigma,\theta}_{\nu jk\ell mn} - L_1(n) \sum_{\nu=1}^{N_x} A^{(1)}_{\ell\nu} P^{\sigma,\theta}_{ijk\nu mn} \\
&- L_2(k) \sum_{\nu=1}^{N_y} A^{(2)}_{j\nu} P^{\sigma,\theta}_{i\nu k\ell mn} - L_2(n) \sum_{\nu=1}^{N_y} A^{(2)}_{m\nu} P^{\sigma,\theta}_{ijk\ell\nu n} \\
&+ L_3(k) \sum_{\nu=1}^{N_z} A^{(3)}_{k\nu} P^{\sigma,\theta}_{ij\nu\ell mn} + L_3(n) \sum_{\nu=1}^{N_z} A^{(3)}_{n\nu} P^{\sigma,\theta}_{ijk\ell m\nu}
\end{aligned}$$

$$+ Q^{\sigma}_{ijk\ell mn} \tag{B.16}$$

$$i\ ,\ \ell = 1,\ldots,\ N_x\ ;\ j,m = 1,\ldots,\ N_y;\ k,\ n = 1,\ldots,\ N_z$$

where the variance function is discretized by

$$P^{\sigma}_{ijk\ell mn} = P(x_i, y_j, z_k, x'_\ell, y'_m, z'_n, t_\sigma) \tag{B.17}$$

Note that (B.16) involves the computation of $P^{\sigma}_{ijk\ell mn}$ which has six subscripts for six spatial coordinate directions. However, it is not difficult to relate the 6-dimensional subscript with the corresponding 2-dimensional matrix subscript by the transformation

$$(i,j,k,\ell,m,n)$$

$$\updownarrow\ (i+N_x(j-1) + N_xN_y(k-1),\ \ell + N_x(m-1) + N_xN_y\ (n-1)) \tag{B.18}$$

It is important to note that this matrix subscripting can be incorporated into efficient FORTRAN implementation. In this way, using the state transition matrix $\Phi(\sigma+1,\sigma)$ of (B.14), it is possible to represent (B.16) in the formal matrix form:

$$\underset{\sim}{P}(\sigma+1) = \underset{\sim}{\Phi}(\sigma+1,\sigma)\underset{\sim}{P}(\sigma) + \underset{\sim}{P}(\sigma)\underset{\sim}{\Phi}^{T}(\sigma+1,\sigma) + \underset{\sim}{Q}(\sigma) \tag{B.19}$$

where $\underset{\sim}{P}(\sigma)$ and $\underset{\sim}{Q}(\sigma)$ are suitably defined $N_xN_yN_z$ x $N_xN_yN_z$ matrices. Note that $\underset{\sim}{P}(\sigma)$ is a symmetric positive semidefinite matrix.

In order to include the effects of numerical errors in the filter design requirements, we utilize the covariance square root implementation (Kaminski et al. (1971)). The covariance square root filter is a data processing algorithm based on a triangular square root factorization of the estimation error covariance matrix and is reputed to be more accurate and stable than the conventional non-square root algorithms. The use of square root matrices implicitly preserves symmetry and assures nonnegative eigenvalues for the computed variance. The square root algorithms achieves accuracy that is compatible with a Kalman filter that uses twice their numerical precision.

Factorization of a symmetric matrix with nonnegative eigenvalues is always possible. As one might expect, the covariance square root is not uniquely determined, however, a unique square root can be defined by a triangular square root matrix. There are three basic algorithms for obtaining the triangular form of the square root matrix. The first, and generally the fastest of the algorithms, employs the Cholesky decomposition. The second algorithm is known as the Householder orthogonalization transformation. This method usually yields more accurate results than the Cholesky decomposition procedure, however, it is considerably slower. The third method is the

modified Gram-Schmidt procedure. The method is comparable to the Householder algorithm with respect to the computation time and accuracy.

The covariance square root matrix $\underset{\sim}{S}(k)$ is defined by

$$\underset{\sim}{S}(k)\underset{\sim}{S}^T(k) = \underset{\sim}{P}(k) \tag{B.20}$$

Then the filter time update equations (B.14) and (B.19) can be summarized in the following covariance square root form:

$$\hat{\underset{\sim}{c}}_-(k+1) = \underset{\sim}{\Phi}(k+1,k)\hat{\underset{\sim}{c}}_+(k) \tag{B.21}$$

$$\underset{\sim}{S}(k+1) = \underset{\sim}{\Phi}(k+1,k)\underset{\sim}{S}_+(k) \tag{B.22}$$

$$\underset{\sim}{S}_-(k+1)\underset{\sim}{S}_-^T(k+1) = \underset{\sim}{S}(k+1)\underset{\sim}{S}^T(k+1) + \underset{\sim}{Q}(k) \tag{B.23}$$

where the subscripts - and + denote the value of the estimate, or covariance square root, at the time immediately prior to and immediately subsequent to the measuring instant, respectively. In the actual computation of (B.22), we apply the same time-splitting technique as (B.8) - (B.10).

(a) Advection part:

$$\delta_t^{1/3} S_{pq}^k = - L_1(k) \sum_{\nu=1}^{N_x} A_{i\nu}^{(1)} S_{\nu_1,q}^{k,\theta} \tag{B.24}$$

$$\delta_t^{1/3} S_{pq}^{k+1/3} = - L_2(k) \sum_{\nu=1}^{N_y} A_{j\nu}^{(2)} S_{\nu_2 q}^{k+1/3,\theta} \tag{B.25}$$

(b) Diffusion part:

$$\delta_t^{1/3} S_{pq}^{k+2/3} = L_3(k) \sum_{\nu=1}^{N_z} A_{k\nu}^{(3)} S_{\nu_3 q}^{k+2/3,\theta} \tag{B.26}$$

where the subscripts are defined by

$$\begin{aligned} p &= i + N_x(j-1) + N_xN_y(k-1) \\ q &= \ell + N_x(m-1) + N_xN_y(n-1) \\ \nu_1 &= \nu + N_x(j-1) + N_xN_y(k-1) \\ \nu_2 &= i + N_x(\nu-1) + N_xN_y(k-1) \\ \nu_3 &= i + N_x(j-1) + N_xN_y(\nu-1) \end{aligned} \tag{B.27}$$

We may note that it is not necessary to compute and store the state transition matrix $\underset{\sim}{\Phi}(k+1,k)$ in the procedure (B.24)-(B.26). As indicated by the subscripts of $\underset{\sim}{S}$, only the matrix multiplication from the left is involved in the computation of the time update factors of $\underset{\sim}{S}$. Thus, different from (B.19), we can arrange a simple and efficient numerical implementation for the time update of covariance square root.

We use a modified Gram-Schmidt orthogonalization procedure in the factorization of (B.23). (For detail see Appendix C.) The modified Gram-Schmidt algorithm is reputed to have accuracy that is comparable with the Householder algorithm. Unlike the classical procedure, the modified algorithm produces almost orthogonal vectors, and reorthogonalization and pivot strategies are unnecessary. From this viewpoint, it is possible to interpret the square root process as a Gram-Schmidt orthogonalization of an appropriately defined state vector.

Using the measurement equation (B.15), define the Cholesky square root matrices $\underset{\sim}{V}(k)$ and $\underset{\sim}{G}(k)$ by

$$\begin{aligned} \underset{\sim}{V}(k) &= \underset{\sim}{R}^{1/2}(k) \\ \underset{\sim}{G}(k) &= [\underset{\sim}{H}(k)\underset{\sim}{S}_{-}(k)\underset{\sim}{S}_{-}^{T}(k)\underset{\sim}{H}^{T}(k) + \underset{\sim}{R}(k)]^{1/2} \end{aligned} \tag{B.28}$$

where the superscript 1/2 is reserved for the Cholesky square root (see Appendix C). Then the filter measurement update equations (A.21) and (A.22) can be summarized in the following covariance square root form:

$$\begin{aligned} \hat{\underset{\sim}{c}}_{+}(k+1) = \hat{\underset{\sim}{c}}_{-}(k+1) &+ \underset{\sim}{S}_{-}(k+1)\underset{\sim}{S}_{-}^{T}(k+1)\underset{\sim}{H}^{T}(k+1)\underset{\sim}{G}^{-T}(k+1)\underset{\sim}{G}^{-1}(k+1) \\ &\cdot[\underset{\sim}{w}(k+1) - \underset{\sim}{H}(k+1)\hat{\underset{\sim}{c}}_{-}(k+1)] \end{aligned} \tag{B.29}$$

$$\begin{aligned} \underset{\sim}{S}_{+}(k+1) &= \underset{\sim}{S}_{-}(k+1) \\ &- \underset{\sim}{S}_{-}(k+1)\underset{\sim}{S}_{-}^{T}(k+1)\underset{\sim}{H}^{T}(k+1)\underset{\sim}{G}^{-T}(k+1)[\underset{\sim}{G}(k+1) + \underset{\sim}{V}(k+1)]^{-1}\underset{\sim}{H}(k+1)\underset{\sim}{S}_{-}(k+1) \end{aligned} \tag{B.30}$$

The filter measurement update equations (B.29) and (B.30) involve Cholesky decomposition of two MxM matrices as depicted in (B.28) and inversion of two triangular Cholesky square roots. Since matrix inversion of the triangular matrix preserves triangularity, this procedure is a costly operation in terms of computer execution time, especially when $M \ll N_x N_y N_z$.

In general, algorithms involving square root matrices reduce the dynamic range of numbers entering into the computations. This factor, together with the greater accuracy that square root algorithms guarantee, directly affects computer word length requirements. A rule of thumb is that square root algorithms can use half the word length required by conventional non-square root

algorithms. The modified Gram-Schmidt triangularization, Cholesky decomposition and its inverse algorithm are described in Appendix C.

C. Square Root Matrix

Factorization of a symmetric matrix with nonnegative eigenvalues (a positive semidefinite matrix) is always possible. Since nxn matrices that are symmetric can be completely described by n(n+1)/2 of their elements, their square roots are not uniquely determined in general. They are, however, related to one another by orthogonal transformations.

If $\underset{\sim}{S}_1$ and $\underset{\sim}{S}_2$ are square roots of a positive semidefinite matrix $\underset{\sim}{P}$, that is,

$$\underset{\sim}{P} = \underset{\sim}{S}_1\underset{\sim}{S}_1^T = \underset{\sim}{S}_2\underset{\sim}{S}_2^T \tag{C.1}$$

then there exists a matrix $\underset{\sim}{T}$ such that

$$\underset{\sim}{S}_2 = \underset{\sim}{S}_1\underset{\sim}{T} \text{ and } \underset{\sim}{T}\underset{\sim}{T}^T = \underset{\sim}{T}^T\underset{\sim}{T} = \underset{\sim}{I} \tag{C.2}$$

in other words, $\underset{\sim}{T}$ is orthogonal. It is important to note that the use of different square root matrices does not alter the results.

Using an upper or lower triangular matrix, a unique square root can be determined since symmetric nxn matrix and triangular nxn matrices are both characterized by n(n+1)/2 of their elements. By computing only the upper or lower triangular nonredundant entries, symmetry and positive semidefiniteness of the covariance matrix are preserved. Upper and lower triangula · factorization involves basically the same techniques and computation tim . Here we summarize the lower triangular factorization of the covariance matrix.

C.1 Lower triangular Cholesky decomposition

Any symmetric positive semidefinite matrix $\underset{\sim}{P}$ has a lower triangular factorization, $\underset{\sim}{P} = \underset{\sim}{S}\underset{\sim}{S}^T$. $\underset{\sim}{S}$ is computed from the following recursive algorithms:

For i = 1,..., n

$$S_{ii} = \sqrt{P_{ii} - \sum_{j=1}^{i-1} S_{ij}^2} \tag{C.3}$$

$$S_{ji} = \begin{cases} 0 & , (j < i) \\ \dfrac{1}{S_{ii}}\left\{P_{ji} - \sum_{k=1}^{i-1} S_{jk}\, S_{ik}\right\}, & (j = i+1,\ldots, n) \end{cases} \tag{C.4}$$

where n = dim P.

C.2 Inversion of lower triangular matrix

Matrix inversion of a lower triangular matrix preserves lower triangularity. $\underset{\sim}{S}^{-1}$ is computed from the following recursive algorithms:

For $i = 1, \ldots, n$

$$S_{ii}^{-1} = 1/S_{ii} \tag{C.5}$$

$$S_{ji}^{-1} = \begin{cases} 0 & (j < i) \\ -\dfrac{1}{S_{jj}} \displaystyle\sum_{k=i}^{j-1} S_{jk} S_{ki}^{-1}, & (j = i+1, \ldots, n) \end{cases} \tag{C.6}$$

C.3 Modified Gram-Schmidt orthogonalization

Let $\underset{\sim}{f}_1, \ldots, \underset{\sim}{f}_n$ be linear independent N vectors with $N \geq n$. Consider the recursions:

For $i = 1, \ldots, n$

$$S_{ii} = \sqrt{\underset{\sim}{f}_i^{(i)T} \underset{\sim}{f}_i^{(i)}} \tag{C.7}$$

$$S_{ij} = \begin{cases} 0 & (j < i) \\ \dfrac{1}{S_{ii}} \underset{\sim}{f}_i^{(i)T} \underset{\sim}{f}_j^{(i)} & (j = i+1, \ldots, n) \end{cases} \tag{C.8}$$

$$\underset{\sim}{f}_j^{(i+1)} = \underset{\sim}{f}_j^{(i)} - S_{ij} \underset{\sim}{f}_i^{(i)} \qquad (j = i+1, \ldots, n) \tag{C.9}$$

Then

$$\begin{bmatrix} \underset{\sim}{f}_1^T \\ \cdot \\ \cdot \\ \cdot \\ \underset{\sim}{f}_n^T \end{bmatrix} [\underset{\sim}{f}_1, \ldots, \underset{\sim}{f}_n] = \underset{\sim\sim}{S}\underset{\sim\sim}{S}^T \tag{C.10}$$

where $\underset{\sim}{S}$ is lower triangular.

Then the factorization (B.23) can be handled by constructing a suitable orthogonal matrix $\underset{\sim}{T}$ such that

$$\underset{\sim}{T}\begin{bmatrix} \underset{\sim}{S}^T(k) \\ \\ \underset{\sim}{W}^T(k) \end{bmatrix} = \begin{bmatrix} \underset{\sim}{S}^T(k) \\ \\ \underset{\sim}{0} \end{bmatrix} \tag{C.11}$$

where

$$\underset{\sim}{W}(k) = \underset{\sim}{Q}^{1/2}(k). \tag{C.12}$$

Using the modified Gram-Schmidt procedure (C.7)-(C.9), the transformation (C.11) can be performed without explicit storage or computation of $\underset{\sim}{T}$.

For the technical details and a more complete discussion of the matrix factorization algorithms we refer the reader to Bierman (1977).

D. Discussion of Approaches to the Design of a Monitoring System

In this Appendix we outline prior approaches that have been proposed for the monitoring system design problem. The object of this Appendi, is to provide the reader with some perspective on other approaches, their advantages and shortcomings, and their comparison with the approach taken here.

Seinfeld (1972) posed the optimal monitoring location problem from the point of view of source surveillance. Given an atmospheric diffusion model he proposed that monitors be located at points where the pollutant concentrations are most sensitive to changes in source emissions. He developed an optimization routine that would automatically find those locations with maximum sensitivity. The results of that work can be viewed as complimentary to those of the present work since we have not considered the criterion of source surveillance here.

Gustafson and Kortanek (1973, 1976) have essentially employed a regression approach to the optimal monitor siting problem. In their 1973 work they propose to determine an optimal regression model by minimizing the differences between observed and calculated concentrations. Let $f(\underset{\sim}{x})$ represent the concentration of a pollutant at location $\underset{\sim}{x}$. The observations can then be represented by $f(\underset{\sim}{x}) + \eta(\underset{\sim}{x})$ where $\eta(\underset{\sim}{x})$ is white, Gaussian noise. The authors propose that $f(\underset{\sim}{x})$ be represented by

$$f(\underset{\sim}{x}) = \sum_{i=1}^{n} a_i \phi_i(\underset{\sim}{x}) + \eta(\underset{\sim}{x}) \tag{D.1}$$

where $\{\phi_i\}$ is an appropriate set of functions, and $\{a_i\}$ are unknown constants. The optimal location problem is posed as determining a set of measurement locations, $\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots, \underset{\sim}{x}_N$, to minimize

$$\sum_{j=1}^{N} p_j \left\{ \sum_{i=1}^{n} a_i \phi_i(\underset{\sim}{x}_j) - f(\underset{\sim}{x}_j) \right\}^2 \qquad (D.2)$$

where p_j are an appropriate set of weighting coefficients.

In more recent work, Gustafson and Kortanek (1976) proposed a scheme based on a least squares fit of sparse measurement data to an analytical dispersion formula. The concentration of a pollutant at location $\underset{\sim}{x}$ is expressed as

$$c(\underset{\sim}{x}) = \sum_{j=1}^{M} q_j v_j(\underset{\sim}{x}) \qquad (D.3)$$

where q_j is the strength of source j, and v_j is the concentration produced at $\underset{\sim}{x}$ by a source of unit strength at source j. Clearly, v_j is a function only of meteorology. If concentrations are measured at N stations at locations, $\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots, \underset{\sim}{x}_N$, yielding measurements $c_1, c_2, \ldots, c_N$, then the authors propose that the M pseudo-source strengths q_j, $j = 1,2,\ldots, M$ can be determined from

$$\sum_{j=1}^{M} q_j v_j(\underset{\sim}{x}_i) = c_i \qquad i = 1,2,\ldots, N \qquad (D.4)$$

The solution to (D.4) for the q_j can be obtained by least squares. Once the q_j have been determined, then they can be used to predict concentrations at other locations for the purpose of choosing new monitoring stations. The key to this approach is that the source strengths are treated as unknown in order to determine the model that is to be used subsequently for siting. This approach is not as desirable as one based on a good source inventory, such as that of Liu et al. (1977).

Hougland and Stephens (1976ab) presented a location model which defines a measure of relationship between an emission source and a potential monitor site. The measures, called coverage factors, are defined for each combination of source, potential monitor, and wind direction. For a tentative assignment of samplers to potential monitor site, a "source oriented sum (SOS)" is calculated. Then a heuristic nonlinear programming technique is used to search for those combinations of sampler assignments that minimize the source oriented sum for the number of monitors allowed on assignment. This model is expressed as follows:

$$\text{Maximize SOS} = \sum_{i=1}^{N_S} \sum_{k=1}^{N_W} \max_{1 \le j \le N_M} \{A_{ijk} X_j\} \qquad (D.5)$$

$$\text{subject to:} \quad \sum_{j=1}^{N_M} X_j = M$$

where: SOS = source oriented sum

i,j,k = indices over N_S sources, N_M potential monitors, and N_W wind directions, respectively

A_{ijk} = coverage factor for source i, wind direction k, and potential monitor site j

M = number of monitors allowed to be assigned to potential sites

$$X_j = \begin{cases} 0 ; & \text{if a sampler is not assigned to potential monitor site j} \\ 1 ; & \text{if a sampler is assigned to potential monitor site j} \end{cases}$$

The contribution of this model is that it defines a source-monitor relationship, it uses this relationship in a optimization scheme for monitor network design, and is a completely source-oriented model.

Vukovich (1976) proposed an objective variational analysis model (OVAM) to establish an optimum sampling network (OSN). If the parameters in the diffusion equation are specified over the urban region, then it is possible to determine the distribution of a particular pollutant using an objective variational analysis model. This technique provides the pollution distribution by making proper use of the sparse measurement data and the governing diffusion equation. Then the representative data is incorporated into a regression model, and combined with the site selection algorithm to yield the optimal sampling network. The criterion that establishes the OSN is the variance function, which yields a measure of the predictability over the area, as well as the correlation and sums of squares of deviations between observed and predicted values. One of the most important steps of the technique is the selection of the regression model.

Buell (1975) proposed a linear regression approach that is basically equivalent to that of Gustafson and Kartanek. It is presumed that there exist a few existing monitoring stations or at least a few points at which observations have been made. On the basis of this given starting network of measurement points, the criterion (D.2) is used to construct the linear regression model and to interpolate concentrations. Using this interpolation

TABLE D.1 SUMMARY OF PREVIOUS APPROACHES TO OPTIMAL AIR POLLUTANT MONITOR SITING

Investigators	Siting Criterion	Comments
Seinfeld (1972)	Locate monitors at points of maximum sensitivity to changes in emission rates from major sources, the "source-surveillance" siting criterion.	Approach based on atmospheric diffusion equation air quality model. Need source inventory and meteorological data for region. Method applicable to inert and reactive pollutants.
Gustafson and Kortanek (1973)	Locate monitors so as to determine an optimal regression fit to the concentration field.	Approach based on statistical optimal experimental design. Regression fit of limited usefulness. Sites sensitive to particular regression expression chosen.
Gustafson and Kortanek (1976)	Construct a model by determining best source strengths to match model to observed data.	Treats source strengths as unknown and determines the best linear model (inert species) to fit the observed concentration data. Once model is formed, additional monitor sites can be selected. Of limited usefulness if actual source inventory is available.
Vukovich (1976)	Fits wind field by objective analysis and then fits a regression model to concentration field.	A more sophisticated variant of Gustafson and Kortanek (1973). Optimal sites chosen on basis of regression model for concentration field. Non-reactive pollutants only.
Hougland and Stephens (1976ab)	Defines a coverage factor that depends on source strength, frequency distribution of wind speed and direction.	Applicable to non-reactive pollutants only.
Liu et al. (1977)	Exercise air quality diffusion model given source inventory and meteorology to produce concentration field. Locate monitors on basis of characteristics of field.	Does not require prior monitoring data. Applicable to inert and reactive pollutants. Best way to approach siting in a region where no stations currently exist.
Buell (1975)	Locate additional monitors at points at which the mean square error of estimates is largest.	A starting network of monitoring stations is assumed. Regression fit of concentrations and interpolation over a region is performed. Optimization is carried out based on a heuristic one-step-at-a-time method. Similar to Gustafson and Kortanek.

of pollutant concentrations over a region, the location of the point yielding the maximum error of estimation is found. This point is then chosen as the best location for a new measurement station. This point is added to the existing observation points. The process is then repeated; the location of the point yielding the maximum mean square error is found, using the new observation station. A second new measurement station is located, etc. In this work, special consideration is given to the calculation of the residual variances or the effects of limited range of influence. The factor analysis method is utilized to specify the residual variances which enter into the diagonal elements of the covariance (or correlation coefficient) matrix.

E. Documentation of Program

E.1 Function

The program accepts a set of monitoring station locations and pollutant concentration data at these stations and produces a grid of estimates of the pollutant concentration. Data cards describing the grid of surface pollutant fluxes, eddy diffusivities, and wind vectors over the region of interest are also required.

E.2 Program Flowsheet and Subroutines

The flowsheet of the program is given in Figure E.1. Subroutines required there are as follows:

COVAC	:	For the time-update computation of the filter square root variance
MGS	:	For the modified Gram-Schmidt orthogonalization procedure
CHOLKY	:	For the Cholesky decomposition procedure
INVTRY	:	For the inverse matrix generation of a triangular square root matrix
FROMM	:	For the Fromm's second-order, zero average phase error finite difference method
TRIG	:	For the solution of an algebraic equation with a triangular coefficient matrix.

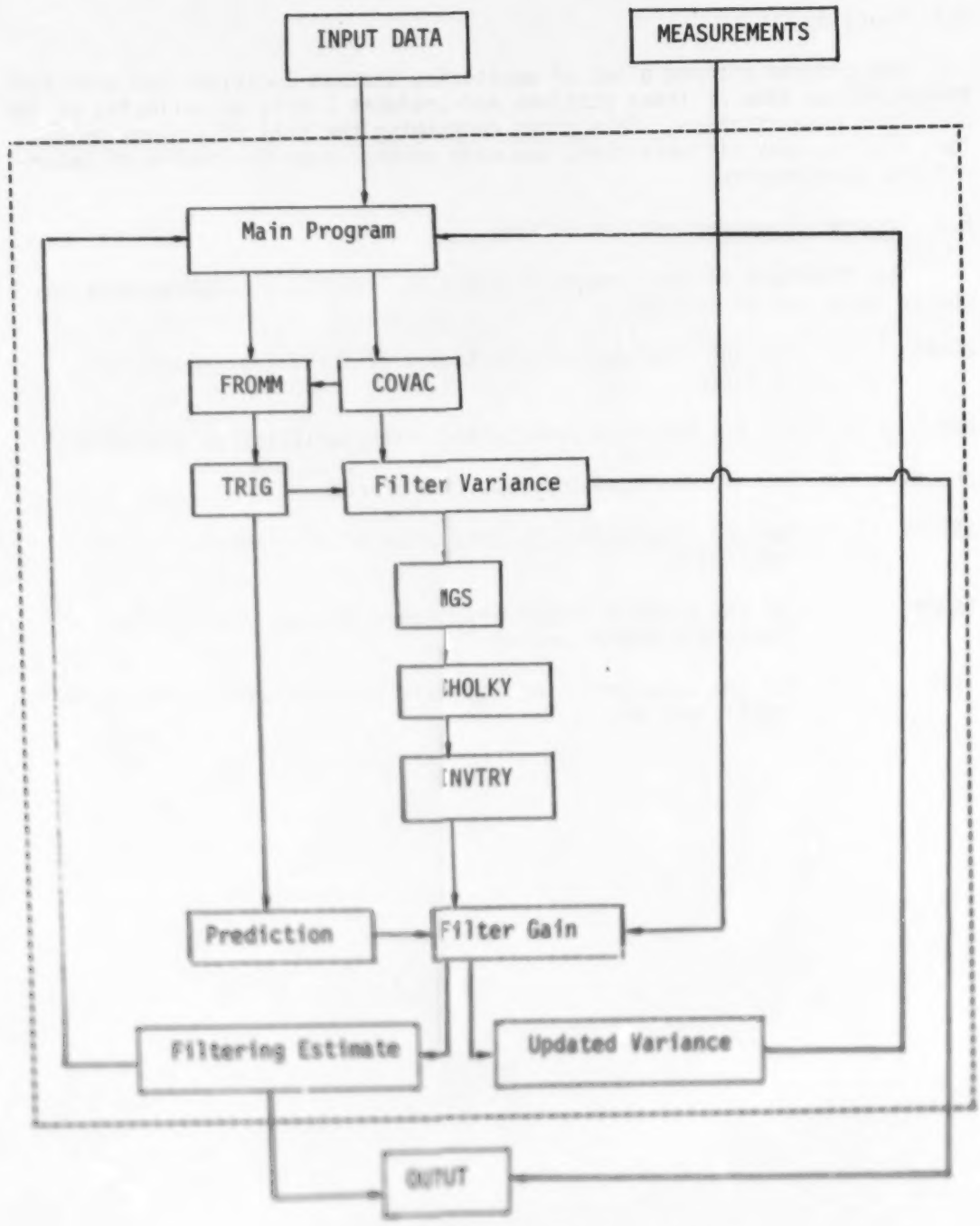

Figure E.1 Flowsheet of the Program

E.3 Input Variables

Definition	Physical Variable	Program Variable	Comment
Filter states	$\hat{c}(x_i,y_j,z_k,t)$	C(I,J,K)	Estimate
	$S_{ij}(t)$	P(I,J)	Square root variance
	$P_{ij}(t)$	PA(I,J)	Filter variance
Mesh conditions	Δx	DX	Mesh spacings
	Δy	DY	
	Δz	DZ	
	Δt	DT	
	N_x	LL	Mesh numbers
	N_y	MM	
	N_z	NN	
Time conditions	t_k	T	
	$t_{k+1}-t_k$	TD	
Measurement conditions	M	NUMBER	Number of stations
	h	EHIT	Effective meas. height

Physical Variable	Program Variable	Input Needed
$c_0(x,y,z)$	C(I,J,K)	C(I,J,K), I = 1,..., LL; J=1,..., MM; K=1,..., NN
$P_0(x,y,z,x',y',z')$	P(I,J)	P(I,J), I, J = 1,..., LL*MM*NN
x_L	IX(L)	IX(L) , L = 1,..., NUMBER
y_L	IY(L)	IY(L), L = 1,..., NUMBER
$\Phi_L(t_R)$	OBS(L,K)	OBS(L,K), L = 1,..., NUMBER, K = 1,...
$S(x,y)$	SOURCE (I,J)	SOURCE (I,J), I = 1,..., LL; J = 1,..., MM
$u(x,y)$	U(I,J)	U(I,J), I = 1,..., LL; J = 1,..., MM
$v(x,y)$	V(I,J)	V(I,J), I = 1,..., LL; J = 1,..., MM
$R_D(z)$	ED(K)	ED(K), K = 1,..., NN
R_{MD}	DK	
$Q(z)$	Q(K)	Q(K), K = 1, ..., NN
R_I	R(I)	R(I), I = 1,..., NUMBER

E.4 Output Variables

Physical Variable	Program Variable	Type of Output
c(x,y,z,t) P(x,y,z,x,y,z,t)	C(I,J,K) PA(I,I)	The computed grid maps are written and/or 3-dimensional perspectives are drawn.

E.5 Error Messages

A warning message is printed by the program when:

1. Negative concentration is calculated. (If C(I,J,K) < - 10.)
2. Too large a concentration is calculated. (OVERFLOW if C(I,J,K) > 10^3.)
3. Too large diagonal entries of the filter variance are calculated (COVARIANCE OVERFLOW if PA(I,I) > 10^{10}.)
4. Too large correlations of the filter variance are calculated. (If PA(I,J)^2 > PA(I,I)*PA(J,J).)

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